PUBLICATIONS

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VOLUME - IV MR 25A-32

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Matphil Reports No. 25A, December 1982
(To appear in two issues of Current Science, 1983)

VECTOR-MATRIX FORMALISM FOR BOOLEAN ALGEBRA AND LOGIC

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SUMMARY

This article deals with the application of the general m x n Boolean vector-matrix representation of the Theory of Relations to Boolean algebra BA-n, with n x n matrices. A new type of relation termed "reverse relation" is defined and it is found vitally important for both Boolean algebra (BA) and logic. In BA, it leads to a new type of non-closure — namely BA-m iteratively leading to a higher BA-n ($n > m$) on reversal. BA-1, associated with propositional calculus (PC), necessarily leads to BA-2 for its full representation, the extended PC which we call as SNS (from syād (Sanskrit) = doubt). This doubtful state is a new state found to be essential for the completeness of PC. BA-3 is shown to be isomorphic to quantif predicate logic (QPL), provided the algebra of connectives is written in terms of what we have designated "canonical stat representable by BA-3 vectors. The algebra of the connectives

Summary (Cont'd)

has 64 "and" ($\mathbb{A}(i, j)$, i, j = 1 to 8) and 64 "or" ($\mathbb{O}(i, j)$ connectives, and a consistent, complete representation of QPL in terms of Boolean vectors, and 3X3 matrices has been worked out. Here again a new basic state "some" (Σ) is found to be essential, in addition to "all" ($\forall$) and "none" (Φ). This state which is there in Ancient Indian Logic of two thousand years ago, makes Godel's second (incompleteness) theorem for QPL understandable from a simple approach.

Vector-Matrix Representation of Boolean Algebras and Application to Extended Predicate Logic (EPL)

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1. Introduction

This article, is in a way, the continuation of the previous article (1) published in this journal. In Ref. 1 the application of Boolean algebras BA-1 and BA-2 to propositional calculus or sentential logic was considered. By trial and error methods, we discovered that the next higher order Boolean algebra (BA-3) is a very suitable one for symbolizing quantified predicate logic and the various connective operators and states that occur in it. When this was done, just as BA-2 led to two new states, D (doubtful) and X (impossible) in addition to T and F, in propositional calculus, a new state, symbolised by $\leq$ (some) was found to be necessary to get a complete set of all states in predic logic, in addition to the usual $\forall$, $\exists$ and their negations. This, however, led to eight possible states by completing the associated BA-3, with four new additions to the standard four that are used in QPL, namely "for all" ($\forall$), "for none" (Φ), "there exists" ($\exists$) and "not for all" (Λ).

Although the requirements of predicate logic could be covered by using these eight states and connective operators (both matrix and non-matrix) as in SNS, it was felt that the full power of the matrix representation can be brought out only by considering a general n-valued logic which can be represented by BA-n. Even further, this BA-n and the matrix operators occurring for it turn out to be still further generalizable by using rectangular matrices of the type $m \times n$ in the theory of relations, connecting m different objects of one type with n different objects of another type. Therefore, this general theory of relations will be considered first. Then its reduction to a system with only $n \times n$ matrices become straightforward. Out of these, the particular cases of BA-1, BA-2 and BA-3 will be discussed, from the general standpoint, and their consequences to logic will then be described. In particular, the applications of BA-3 to quantified predicate logic turn out to be very novel and these will be described in some detail.

2. Theory of Relations and Boolean Matrices

To keep the tenor of this article at an elementary level, we shall illustrate the method of applying Boolean vectors and matrices for the Theory of Relations by means of a simple example, although general proofs of the statements we make can be readily formulated. We take two sets, — one designated P ($= p_1 , p_2 , p_3 , p_4$) consisting of 4 parents and the other designated C ($= c_1 , c_2 , c_3 , c_4 , c_5$) consisting of 5 children. The forward relation from parent to child, which we may denote by $\underset{\sim}{C}$ (standing for "child of") is representable by a "truth table", as in Table 1, in which, an entry 1 or 0 as C_{ij} means that the relation exists, or is absent between c_i and p_j . Thus, c_3 is the child of p_1 and p_2, while c_1 and c_2 are children of p_3 and c_4 of p_4; c_5 is not the child of any of p_1 to p_4 , although it is included in the set $C \equiv \{c_j\}$. Similarly, for the relation "parent of", $\underset{\sim}{P}$.

Table 1. Truth tables for parent-child relationships

The relations in Tables 1(a) and (b) can be written as Eqns (1a) and (1b) below. In this, the row vectors $\langle p|$ and $\langle c|$ stand for the Boolean vector representation of which constituents are present. Thus, the state vector (1 0 1 1) for $\langle p|$ indicates that p_1, p_3, p_4 are

Table 1. Truth tables for parent-child relationships

(a) $\underset{\sim}{C}$ (Child of)

	c_1	c_2	c_3	c_4	c_5
p_1	0	0	1	0	0
p_2	0	0	1	0	0
p_3	1	1	0	0	0
p_4	0	0	0	1	0

(b) $\underset{\sim}{P}$ (parent of)

	p_1	p_2	p_3	p_4
c_1	0	0	1	0
c_2	0	0	1	0
c_3	1	1	0	0
c_4	0	0	0	1
c_5	0	0	0	0

present and p_2 is absent. Then, the relational matrices in (1a) and (1b) are exactly as given in the two tables, namely 5X4 for $|C|$ and 4X5 for $|P|$. Thus, we have

$$\langle p|\,C\,| = \langle c| \quad , \text{ for Table (1a)} \tag{1a}$$

$$\langle c|\,P\,| = \langle p| \quad , \text{ for Table (1b)} \tag{1b}$$

It is obvious that the matrices $|C|$ and $|P|$ are transposes of one another, and they represent the two relations in (1a) and (1b), which are termed "reverses" of each other. The relation $\underline{a}\,\underset{\sim}{R}\,\underline{b}$ read in the "reverse" direction as $\underline{b}\,\underset{\sim}{R}'\,\underline{a}$ has as its matrix $|R'| = |R^t|$, the superscript 't' standing for "transpose".

The notation of a row vector as a "bra" vector ($\langle v|$), a column vector as a "ket" vector ($|v\rangle$) and the relational matrix enclosed by two vertical lines (as in $|Z|$), follows the Dirac bracket notation in quantum mechanics (see [1] , for fuller details). We write all equations from left to right, as this is the order in which logical relations are expressed — as in "$\underline{a}$ implies $\underline{b}$" ($\underline{a} \Longrightarrow \underline{b}$), which has the notation $\underline{a}\,\underset{\sim}{I} = \underline{b}$ in our nomenclature (see [1]), with $\langle a|$ and $\langle b|$ as 2-element boolean bra vectors and $|I|$ as a 2X2 boolean matrix, giving $\langle a|I| = \langle b|$.

We shall discuss two practical uses of relational matrices that are relevant to logic and Boolean algebra.

(a) Unary relation and its reverse: If $\langle p'|$ is the Boolean vector representing a (partial) ensemble of the full set $\{p_i\}$, e.g. (1 0 0 1), we may ask the question, "which c_j's are present, among the children, of the two parents p_1 and p_4 of this $\underline{p}'$-ensemble?" The answer is given as the Boolean vector $\langle c'|$ in Eqn. (2a), which, for $\langle p'|$ = (1 0 0 yields $\langle c'|$ = (0 0 1 1 0) as in (2b) — namely, only the two children c_3 and c_4.

$$\langle p'| \; C \; | = \langle c'| \tag{2a}$$

and

$$\langle p'| = (1 \;\; 0 \;\; 0 \;\; 1) \longmapsto \langle c'| = (0 \;\; 0 \;\; 1 \;\; 1 \;\; 0) \tag{2b}$$

Note that all the additions and multiplications involved in the vector-matrix product are as per standard Boolean algebra BA-1 (see [1] for more examples), where the matrix $|C|$ is explicitly as shown below in (3a). The meaning and use of the matrix $|C^c|$ in (3b) will be clear in Section 2(ii).

$$|C| = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \tag{3a}$$

$$; \; |C^c| = \begin{pmatrix} 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \end{pmatrix} \tag{3b}$$

In the same problem, if the question is reversed, with $\langle c'|$ as input, we obtain Eqn. (4a), yielding the vector $\langle p''|$ as given by (4b).

$$\langle c'|\ P\ | = \langle p''| \qquad (4a)\ ; \qquad \langle p''| = (1\ \ 1\ \ 0\ \ 1) \qquad (4b)$$

The interesting feature of this reversal of the relation $\underset{\sim}{C}$ to the reverse relation $\underset{\sim}{P}$ is that $\langle p''|$ in (4b) is not the same as $\langle p'|$ in (2b). The reason, in this particular case, is that c_3 is the son of p_1, but both the parents p_1 and p_2 are present in the set $\{p_i\}$. One parent (p_1) gives the child (c_3) in the forward direction using the relation $\underset{\sim}{C}$, but in the reverse direction, the relation $\underset{\sim}{P}$ applied to the same child (c_3) gives <u>both</u> the parent p_1 and p_2, — in general the maximal ensemble of parents possible. Thus, the 'reverse' relation does not have the nature of 'inverse' in ordinary algebra and the matrix $|Z|$ goes over into its <u>transpose</u> $|Z^t|$, on reversing the relation. This property of <u>transpose representing reversal of a relation</u> is vitally important for our applications of Boolean vectors and matrices to logic.

(b) <u>Dirac (matrix) product;</u> Suppose, in Table 1a, we take the first of the above two examples and work out the Dirac product $\langle p'|\ P\ |\ c'\rangle$, as defined in [1], which is repeated

as (5) below for ready reference

$$\langle a \mid Z \mid b \rangle = \sum_i \sum_j a_i Z_{ij} b_j = k_\alpha \text{ , a scalar} \qquad (5)$$

In this, the value of k_α can only be 0 or 1 in Boolean algebra (the need for the subscript α in k_α will be clear in Eqn. (7) below). If $k_\alpha = 1$, it means that the answer to the question "Is there at least one a_i and one b_j in the ensembles $\underline{a}$ and $\underline{b}$, that are related by the relation $\underset{\sim}{Z}$?" is "yes". Similarly, $k_\alpha = 0$ means that the relation $\underset{\sim}{Z}$ does not connect any a_i with any b_j in the two ensembles represented by $\langle a|$ and $\langle b|$, that are provided.

In the same way, we may form a Dirac product using the complement of $|Z|$, namely $|Z^c|$, where

$$Z^c_{ij} = | - Z_{ij} \text{ , its complement in BA-1} \qquad (6)$$

The matrix $|Z^c|$ represents the "non-relation" of $\underset{\sim}{Z}$, so that if there is 1 in position (i, j) in $|Z^c|$, then a_i and b_j are non-related by the relation $\underset{\sim}{Z}$. We thus have an equation similar to (5) for k_β, namely

$$\langle a \mid Z^c \mid b \rangle = \sum_i \sum_j a_i Z^c_{ij} b_j = k_\beta \qquad (7)$$

and the properties of k_β for $\underset{\sim}{Z}^c$ are the same as those of k_α

(c)
(iii) Binary relation expressed via Dirac products: We now consider the truth value of the binary relation $\underline{\underline{a}}\ \underset{\sim}{Z}\ \underline{\underline{b}}$, expressed via the state vectors $\langle a|$, and $\langle b|$, and the matrix $|Z|$ representing the relation $\underset{\sim}{Z}$, and its derived complement $|Z^c|$. The truth value of the relation is expressible in terms of two Boolean scalars k_α and k_β, which form a Boolean 2-vector $(k_\alpha \quad k_\beta)$. In order to see the various possibilities, three examples can be taken, as in Sl. Nos 1, 2, 3 of Table 2.

Table 2. Dirac product values for four typical examples of the relation C.

Thus, the non-relation $(\underset{\sim}{C}^c)$ does not exist for the Row 1, and the relation $(\underset{\sim}{C})$ exists, while the opposite is the case of Row 2 of Table 2. We shall say that the truth value is "true" (T) for the former, and "false" (F) for the latter, which agrees with the idea that only one of the two — "relation $\underset{\sim}{C}$" or "non-relation $\underset{\sim}{C}^c$" exists for these cases. We represent these by the Boolean vectors (1 0) and (0 1) respectively, as in SNS (see Ref. [1]).

However, it is possible that both $\underset{\sim}{C}$ and $\underset{\sim}{C}^c$ are not absent (Row 3 of Table 2). This gives $(c_\alpha \quad c_\beta) = (1 \quad 1)$, when

Table 2. Dirac product values for four typical examples of the relation $\underset{\sim}{C}$.

Sl. no.	$\langle p' \rvert$	$\langle c' \rvert$	k_α	k_β	Logical State $\underset{=}{k} = (k_\alpha \quad k_\beta)$ of the relation $\underset{\sim}{C}$
1	(0 0 1 0)	(1 1 0 0 0)	1	0	T
2	(0 0 1 1)	(0 0 1 0 1)	0	1	F
3	(1 0 0 1)	(0 0 1 1 0)	1	1	D
4	(0 0 0 0)	(any values)	0	0	X

state of $\underline{p}\ \underset{\sim}{C}\ \underline{c}$ is "indefinite" (D, standing for "doubtful"). Row 4 shows one more example, namely of both the relations $\underset{\sim}{C}$ and $\underset{\sim}{C}^c$ being non-existent. It is easy to show that such a situation will occur only if either the vector $\langle p'|$ or $\langle c'|$ is zero for all its components, when a relation between $\underline{p}$ and $\underline{q}$ is "impossible" — represented by (0 0). The letter X indicates this state.

(d)
(iv) Summary of Section 2: Thus, the truth value of a binary relation requires a BA-2 representation with two scalars in the form of Dirac products so that the relation $\underline{a}\ \underset{\sim}{C}\ \underline{b} = \underline{c}$ becomes representable as (8a) and (8b):

$$\underline{a}\ \underset{\sim}{C}\ \underline{b} \longleftrightarrow (a\,|\,C\,|\,b) = (c_\alpha\ \ c_\beta) = \quad \text{(say)} \qquad (8a)$$

where c_α and c_β are given by the Dirac products

$$\langle a\,|\,C\,|\,b\rangle = c_\alpha\ ; \quad \langle a\,|\,C^c\,|\,b\rangle = c_\beta \qquad (8b)$$

We shall use $(a|C|b)$ to indicate the SNS state $(c_\alpha\ \ c_\beta)$ of $\underline{a}\ \underset{\sim}{C}\ \underline{b} = \underline{c}$. Also, since the matrix $|C^c|^c = |C|$ itself, the bracket giving the truth value for the relation $\underline{a}\ \underset{\sim}{C}^c\ \underline{b}$ is

$$(a|C^c|b) = (c_\beta\ \ c_\alpha) = \underline{d} = \quad \in \underset{\sim}{N} \qquad (8c)$$

where c_α and c_β are the same as in (8b) (See [1] for the definition of SNS region $\underset{\sim}{N}$).

Obviously, the matrix $|C|$ of (8a) can be written as $|C| = \sum_{\lambda} \sum_{\mu} |C_{\lambda\mu}|$ such that each $|C_{\lambda\mu}|$ has only one non-zero element at location (λ, μ) in the matrix. Such a matrix $|C_{\lambda\mu}|$, with a single 1 in it, may be called a "singular matrix" In terms of these, we have

$$(a|C|b) = \sum_{\lambda} \sum_{\mu} (a|C_{\lambda\mu}|b) \qquad (8d)$$

The use of such singular matrices in quantified predicate logic is to be found in Sections 6. //

3. Types of Relations in Boolean Algebra

(a) Reversal of a relation, in general: The above general treatment of a relation $\underset{\sim}{Z}$ expressible by an m x n Boolean matrix, can be seen to be fully acceptable within the range of the mathematics of set theory, Boolean algebra and matrix theory. However, when the above formulae are applied to logic, they lead to extremely interesting results. Some of them turn out to be quite novel, not only in leading to simplified procedures in the mathematical treatment of the theory of logic, but even to some new concepts in logic itself.

The concept of the "reversal" of relations does not appear to be generally recognized in the literature. We saw

one aspect of it connected with unary relations earlier in subsection 2(i), Eqs (2b) and (4b). Thus the ensemble $\langle p'| = (1 \quad 0 \quad 0 \quad 1)$ of parents gave the ensemble $\langle c'| = (0 \quad 0 \quad 1 \quad 1 \quad 0)$ for children; but when the operation was reversed, we obtained $\langle p''|$ as $(1 \quad 1 \quad 0 \quad 1)$, different from $\langle p'|$. It can be shown that $\langle p''|$ is really the set of "all possible" parents of the children $\langle c'|$, and that the members of $\langle p'|$ are <u>included</u> in $\langle p''|$. This idea that a Boolean vector-matrix operation gives the maximal set of members contained in the vector generated by it, is a very important one for our discussion. The ensemble of elements like $\langle p'|$ and $\langle c'|$ form a '<u>lattice</u>' of abstract algebra. In fact Boolean algebras form "fully complemented distributive lattices" (See [2]).

<u>(b) Reversal of binary relations</u>: We now consider the technique of reversing a binary relation. We start with 8(a, b, c). For this, we suppose that the state of the vector $\underline{c} = (c_\alpha \quad c_\beta)$ is given and so also is the relation $\underline{\zeta}$. We are then required to find out the state that can be deduced for $\langle b|$ given that of $\langle a|$, or <u>vice versa</u> . Taking the former first, the relation between $\underline{a}$ and $\underline{b}$ can be given, in general, in terms of Boolean vector-matrix products involving the matrices $|C|$ and $|C^c|$, as in Eqns (9a to d) :

$\underline{c} = T$ yields $\langle a|C| \otimes (\langle a|C^c|)^c = \langle b|$ (9a)

$\underline{c} = F$ yields $\langle a|C^c| \otimes (\langle a|C|)^c = \langle b|$ (9b)

$\underline{c} = D$ yields $\langle a|C| \oplus \langle a|C^c| = \langle \underset{\sim}{1}|$ (9c)

$\underline{c} = X$ yields $\langle b| = \langle Q|$, and $\langle a| = \langle \underset{\sim}{Q}|$ (9d)

(In (9c, d), $\langle \underset{\sim}{1}|$ stands for a state vector with 1 for all components, and $\langle \underset{\sim}{Q}|$ for one with 0 for all the components.

In these equations, it is important to remember that, in general, the vectors $\langle a|Z| = \langle d|$ and $\langle a|Z^c| = \langle c|$ are not complementary to one another, and $\langle d|e\rangle$ need not be a null vector. Secondly, the vector $\langle b|$ yielded by the l.h.s's of (9a), or (9b) is what may be called the "maximal" vector, containing all possible elements b_i which can be non-zero. In an actual case, the vector $\langle b'|$ can have 1's for any, or all, of the b_i's in the maximal vector $\langle b|$; but not all b_i's can be zero (which will correspond to the case of $\underline{c} = X$ of (9d)). In this sense, the vital factor in each of (9 a) and (9b) is the second of the two terms joined by the boolean product and the first term only selects out of these, those that go into the vector $\langle b|$.

On the other hand, in (9c) the result for $\langle b|$ is $\langle \underset{\sim}{1}|$, which stands for the vector containing unities for all the elements b_i ($i = 1$ to n) of the vector $\langle b|$ — namely (1 1 1 . . . 1), corresponding to the full set. In the same way, if $\underline{c} = X$, as in (9d), the vector $\langle b|$ is $\langle \underset{\sim}{0}|$, which, indicates that the set B represented by $\langle b|$ is a null set.

(c)
(~~iii~~) Boolean addition and multiplication of vectors: Since the n generators of BA-n are non-intersecting and one is not included in the other, the corresponding vectors form a basic set $\langle a_i|$, $i = 1$ to n, for the algebra. In the standard formulation of Boolean algebra (see e.g. [2]), as a special type of lattice, the only relations through which these can combine are via the operations of boolean addition $\oplus$ and Boolean multiplication $\otimes$ (both of which are distributive with respect to one another), leading to the equations

$$\langle a| \oplus \langle b| = \langle c| \iff a_i \oplus b_i = c_i \,, \quad i = 1 \text{ to } n \qquad (10)$$

$$\langle a| \otimes \langle b| = \langle d| \iff a_i \otimes b_i = d_i \,, \quad i = 1 \text{ to } n \qquad (11)$$

All the axioms of boolean algebra are satisfied by the n-vector representation, if it is noted that complement $\langle a^c|$ of $\langle a|$

can be defined by

$$\langle a^c| = (a_1^c , \ldots a_i^c \ldots a_n^c), \qquad (12a)$$

where ... $$a_i^c = 1 - a_i \qquad (12b)$$

and the set of all 2^n vectors of BA-n is closed with respect to the application of the operations in (10), (11), and (12).

As regards matrix multiplications of the type we have envisaged in Section 2 (namely by $n \times n$ matrices in BA-n), they employ only the types of elementary operations characteristic of BA-1, via $\oplus$ and $\otimes$, applied to 1 and 0 of this algebra. Hence, the set of 2^n vectors of BA-n is closed with respect to the operations of these Boolean matrix multiplications also. However, with respect to its applicatic to logic, Boolean matrix operators and the symbolic Boolean operators of BA's, have entirely different interpretations, as will be shown below (See Sections 6 (k), (e), (f)).

(d)
(iv) Closure of Boolean algebras: The reversal of the binary relation. $(a \mid Z \mid b) = \underline{c} = (c_\alpha \quad c_\beta)$, may be symbolically represented by

$$(c| \overleftarrow{Z} | a) = \langle b| \quad \text{(given } c_\alpha \text{ , } c_\beta \text{ and } \langle a|) \qquad (13)$$

Eqn. (8) has also another reverse, denoted by the operator $\overleftarrow{\underset{\sim}{Z}}^t$, connecting $\underline{c}$ and $\langle b|$ to give $\langle a|$, the corresponding matrix being $|Z^t|$. Similar to (13), we can write this relation as

$$(c|\overleftarrow{Z}^t|b) = \langle a| \quad (\text{given } c_\alpha, c_\beta \text{ and } \langle b|) \qquad (14)$$

Since reversals of matrix operators representing binary relations yield only vectors contained in the Boolean algebra, the algebra is closed with respect to these also. On the other hand, the algebra is not closed when the Boolean operations $\oplus$ and $\otimes$ are reversed. This is not discussed here, but the consequences are indicated for the particular case of BA-2, in ~~Section~~ [1], and its generalization is indicated there.

4. Vector-matrix Formalism Applied to Propositional Calculus

This aspect has been discussed in the previous paper [1] and will not be considered in detail here. We shall only comment on the fact that BA-1 readily represents the classical sentential calculus as discussed in standard books on logic (e.g. [2], [4]), while BA-2 is needed for its extended form, namely SNS. It may be mentioned that the matrices discussed in the previous section for the theory of relations are in

general rectangular (m x n), but for Boolean algebra of genus-n (BA-n), the number of states possible is n for all entities, and hence it is representable by n-element vectors and n x n square matrices. The other formulae in the previous two sections are unaltered.

SNS has four states T, F, D, X corresponding to the four different vectors (1 0), (0 1), (1 1) and (0 0) of BA-2. This set of states is closed with respect to 2X2 Boolean matrix multiplications, i.e. logical relations of the forward type. From equation (9a-d), it is easy to show that reverse relations corresponding to all the 16 matrix operators also lead to one of the four states, represented by these vectors. This can be taken as a proof of the closure of propositional logic.

On the other hand, when the standard Boolean algebraic connectives $\oplus$ and $\otimes$ are applied to SNS, they lead again only to one of the four states, as shown in Table 3. In this case, when reverse operations are considered for these two logical operators which have been given the name "unanimity" ($\underset{\sim}{U}$) and "vidya" ($\underset{\sim}{V}$), something not contained in BA-2 is produced. These operators are the same as $\underset{\sim}{Q}$ and $\underset{\sim}{A}$

for PC with BA-1 representation, but are quite different when applied to the four states of SNS. In fact, $\underset{\approx}{U}$ and $\underset{\approx}{V}$ are not the same as "or" and "and" in SNS, and lead to 4X4 truth tables, and produce states outside even BA-2 on reversal.

In order to illustrate how such a state outside BA-2 occurs when a relation $\underline{a} \underset{\approx}{V} \underline{b} = \underline{c}$ is reversed, we shall consider the case where $\underline{c} = T$ and $\underline{a} = T$, and we ask, "What is $\underline{c} \underset{\approx}{V} \underline{a} = \underline{b}$?" This is readily answered by looking at Table 3, and we get the state "T or D, but not F". Similarly, we can also obtain "F or D but not T", from the application of the reverse $\overset{\leftarrow}{\underset{\approx}{V}}$ operator. If these two are combined by the connective $\underset{\approx}{V}$, we obtain the state "D, but neither T nor F", whose complement is "T or F, but not D". We thus obtain four new states in addition to the four standard states T, F, D, X isomorphic to BA-2. These give a total of eight ($= 2^3$) states, which can be shown to be isomorphic to the 8 states of BA-3.

Therefore, if the Boolean operators $\oplus$ and $\otimes$ are reversed in BA-2, we get not only states occurring in BA-2, but also four others, leading to a complete set of states of BA-3.

Table 3. Truth tables for unanimity ($\underset{\approx}{U}$) and vidya($\underset{\approx}{V}$) worked out using the algebra of BA-2

Table 3. Truth tables for unanimity ($\underset{\sim}{U}$) and vidya($\underset{\sim}{V}$) worked out using the algebra of BA-2

(a) $\underset{\equiv}{a}' \underset{\sim}{V} \underset{\equiv}{a}'' = \underset{\equiv}{a}^*$

$\underset{\equiv}{a}'$ \ $\underset{\equiv}{a}''$	T	F	D	X
T	T	X	T	X
F	X	F	F	X
D	T	F	D	X
X	X	X	X	X

$^* \underset{\sim}{V} \equiv \otimes$

(b) $\underset{\equiv}{a}' \underset{\sim}{U} \underset{\equiv}{a}'' = \underset{\equiv}{a}^\dagger$

$\underset{\equiv}{a}'$ \ $\underset{\equiv}{a}''$	T	F	D	X
T	T	D	D	T
F	D	F	D	F
D	D	D	D	D
X	T	F	D	X

$^\dagger \underset{\sim}{U} \equiv \oplus$

(a) Property of closure of Boolean algebras including reverse operations.

Just as BA-2 with $3(= 2^2 - 1)$ non-impossible elements leads, by binary reversal of the operation of Boolean x, to BA-3 with $2^2 - 1 (= 3)$ generators and $7(= 2^3 - 1)$ non-impossible elements, the process can be extended to give a series of BA-n's successively, with $n = 7$, $n'(= 2^7 - 1)$, $n''(= 2^{n'} - 1)$ etc. generators, producing an infinite sequence of Boolean algebras (BA-n) with $n = 2, 3, 7, n', n''$, etc, going upto an infinite value for n. Hence, if "reversal" of all relations is an admissible operation (similar to "inverse" in ordinary algebra, group theory etc.), then, Boolean rings (BA-n) with $n = 2, 3, 7..$ are inter-related, and any one leads necessarily to the next higher one, on including the results of reversing the relations in the earlier one.

Thus, if a completely closed Boolean algebraic system is at all possible, it must necessarily have an infinite number of elements. This is similar, for example, to the set of positive integers which has no last member, although every member of it can be described and mathematically utilized, in principle. We believe that this new concept of non-closure of Boolean algebras of finite order (2^n), has not

been pointed out earlier in connection with studies on Boolean algebra.

However, if only matrix reversals are demanded (but not reversals of the Boolean operations ⊕ and ⊗ in BA-n), then the Boolean algebra generated by n basic vectors in our vector-matrix formalism is complete and closed. This general theorem for BA-n has its repurcusions in showing that bA-2 and BA-3, which can represent, according to us, PC and QPL of logic, are complete and closed, even including unary reversal and binary matrix reversal. This theorem regarding BA-n indicates that logic as it is normally understood is essentially a closed system. The only way it is open and leads on to a higher order from any BA-n is via the reversal of the forward operations of ⊕ and ⊗ in that BA-n system.

Thus Boolean algebra, mathematical logic, and Boolean vector-matrix formalism, are all isomorphic with one another and many theorems regarding logic can be derived from the representation — and this makes thinking and logical analysis much more easy.

5. Essentials of QPL with reference to BA-3

(a) Standard QPL states

The two quantifiers that are used in the standard theory of QPL are "for all" ($\forall$ x) and "there exists" ($\exists$ x). These "quantify" the sentential predicate, which we may denote, for the variable x, by ($\underline{s}$ x) with $\underline{s}$ standing, in general, for "sentence". There is also a third entity, that is applied in front of the quantifier, which has two states, corresponding to an affirmation or a negation of the quantifier. We suggest the name "sign" for this and use the symbol $\rightleftharpoons$ to denote negation — e.g. $\rightleftharpoons(\forall x)\ (\underline{a}\ x \Longrightarrow \underline{b}\ x)$ or $\rightleftharpoons(\exists x)\ (\underline{a}\ x\ \&\ \underline{b}$ The negation of the sentence $\underline{s}$, where necessary, is indicated by the PC or SNS negation symbol $\neg$ before $\underline{s}$. However, the eight quantified forms that are obtained using $(\forall x)$, $(\exists x)$, $\neg$ and $\rightleftharpoons$ are not independent. They form four pairs of equivalent statements, as given in (15a to d).

$$(\forall x)\ (\underline{s}\ x) \;=\; \rightleftharpoons(\exists x)\ (\neg \underline{s}\ x) \qquad (15a)$$

$$\rightleftharpoons(\forall x)\ (\underline{s}\ x) \;=\; (\exists x)\ (\neg \underline{s}\ x) \qquad (15b)$$

$$(\forall x)\ (\neg \underline{s}\ x) \;=\; \rightleftharpoons(\exists x)\ (\underline{s}\ x) \qquad (15c)$$

$$\rightleftharpoons(\forall x)\ (\neg \underline{s}\ x) \;=\; (\exists x)\ (\underline{s}\ x) \qquad (15d)$$

The quantifier "for none" ($\nexists$ x), standing for "not there exists"

viz. $\neg(\exists x)$, is used quite often, and this suggests that we must coin a symbol also for "not for all", and we employ (Λx) for this, standing for $\neg(\forall x)$.

We have used two different symbols $\neg$ and $\bar{}$ in the above examples, and these two have entirely different algebraic properties, although they both have only two states— namely "yes" and "no". The former negates only the state of the quantifier — e.g. $\neg(\forall x)$ means "not for all" and not "for all, not". The latter acts only on $\underline{s}\, x$. The two are interrelated (see later for precise details). Thus we have —

$$(\forall x)(\underline{s}\, x) = (\exists x)(\bar{\underline{s}}\, x) \qquad (16a)$$

$$(\forall x)(\bar{}\,\underline{s}\, x) = (\dot{\Phi} x)(\underline{s}\, x) \qquad (16b)$$

The second of these demands that <u>every</u> x has the property "not $\underline{s}$ x", while the first only requires that there are <u>some</u> x's having the property "not $\underline{s}$ x".

A little reflection will show that the state $(\forall x)$ is implicitly assumed in every statement of propositional calculus, without mentioning any particular quantifier state

with reference to it. Thus "men are mortal" is equivalent to saying, "all men are mortal". We will find this property of $(\forall x)$ that it is an unstated quantifier of propositional calculus very useful in deriving relations between statements in PC and statements in QPL [8].

(b) Boolean vector representation of standard QPL states

The statements of QPL in the standard form, such as those in (15) and (16) can be represented via BA-1, BA-2 and BA-3 vectors as follows:

(i) We use SNS for $\underset{\sim}{s}\, x$ which is a statement in PC, and this requires two symbols s_α and s_β, written simply as $(\alpha\ \beta)$, for defining it, with four truth values T, F, D, X. The ~~strong~~ negation operator for $\underset{\sim}{s}\, x$ is the SNS operator $\underset{\sim}{N}$ corresponding to the BA-2 matrix $|N|$ (see [1]).

(ii) As will be clear from the discussions in the next section, we find an absolute need for BA-3 to represent the quantifier. Although we have needed so far, in our discussions, only four quantifier states $\forall, \exists, \underset{\sim}{\exists}, \Lambda$, they do not form a complete Boolean algebra of any genus, and are properly represented only in BA-3. Preliminary studies indicated that their properties are representable by the BA-3 vectors ~~given~~

In (17):

$\forall = (1\ 0\ 0)$, $\exists = (1\ 1\ 0)$, $\Phi = (0\ 0\ 1)$, $\Lambda = (0\ 1\ 1)$

Simultaneously, the other negation operator $\neg$ is the BA-3 complementation operator ($\sim$), whose effects we denote by a superscript ^{c}, or, as will be seen in the next section, by the operator $\mathbb{M}$. The effects of this operator is to change 1 to 0 and 0 to 1 in all the three vector components q_γ, q_δ, q_ϵ of the quantifier $Q_{\gamma'}$, written as (γ' δ' ϵ'). It is readily verified that

$$\forall^c = \Lambda, \quad \Lambda^c = \forall, \quad \exists^c = \Phi, \quad \Phi^c = \exists \qquad (1$$

(The reason for the primes in γ', δ', ϵ' is to distinguish the quantifier in the standard form from that in the canonical form which will be defined in subsection (c) below.)

(iii) We shall use an one-element vector ($\hat{S}$) to denote the "sign" of the standard form, associated with the negation symbol $\neg$. Thus $\hat{S} = 1$ indicates affirmation and $\hat{S} = 0$ indicates negation of the quantifier.

With the above definitions, a quantified state $Q_{\gamma'}$ in QPL, expressed in the standard form adopted in all textbooks requires six parameters $(q_{\hat{S}})$, $(q_{\gamma'}\ q_{\delta'}\ q_{\epsilon'})$ $(q_\alpha\ q_\beta)$ to

represent it. In this, every one of the components from q_α to q_ζ is a Boolean variable in BA-1, having only two possible values 1 and 0. Where convenient, we shall represent the state in the "standard"-form by $(\hat{\S})\ (\nu'\ \S'\ \epsilon')\ (\alpha\ \beta)$, in which the primes for ν, $\S$, ϵ are used to distinguish this from the "canonical" form $(\nu\ \delta\ \epsilon)$ discussed in the next subsection.

It would appear, from the 6-element description of $\mathcal{Q}'$ in the standard format, that there are $2^6 = 64$ possible different quantified states. Actually this is not so and only eight of them are distinct, out of which four cover all the standard quantified states employed in the literature for standard QPL. These features are described in the next subsection 5(c), where we shall use the term "extended" QPL (EQPL) if it is necessary to draw attention to the extra four non-standard states of BA-3 specifically.

(c) Interrelations between standard QPL states: Out of the 64 possible standard forms, 16 are especially interesting in that the treatment of quantified predicate logic in the literature is based only on these, just as propositional calculus uses only two states T and F in the standard literature, while

we find the need for two more states D and X, when reverse relations are taken into account. These 16 can be obtained by taking the four quantifier states ($\forall x$), ($/\!\backslash x$), ($\rceil x$) ($\bar{\Phi} x$) and attaching, in front and after the quantifier symbol, the BA-1 symbols $\neg$ and $\neg$ where necessary. Table 4 below lists these 16 different forms in QPL, of which there are four equivalent forms of each of the states, which are interrelated to one another by four equivalence operators, called "modifiers" $\mathcal{E}_E$, $\mathcal{E}_N$, $\mathcal{E}_M$, $\mathcal{E}_L$.

Table 4 The sixteen different forms in standard QPL obtainable from $\forall$ and $\exists$ and their interrelationships.

In each row of this table, there is just one entry which does not have negation either for the sign or for the sentence. In this particular form (enclosed in a box), the ~~sentence is~~ occurs the affirmative sense for the quantifier and the sentence, and hence we abstract the quantifier part alone of this, and use it for the name of the full quantifier predicate state, which is represented, in the standard form, by all the four entries in that row, and which are logically equivalent to one another. This is shown in the ~~first~~ second column of the table which requires only three components V , δ , ϵ . We name this symbol as the

Table 4. The sixteen different forms in standard QPL obtainable from $\forall$ and $\exists$ and their interrelationships.

Canonical form $(\gamma\ \delta\ \epsilon)$	Modifier used for translation and standard form			
	$\mathcal{E}_E$	$\mathcal{E}_N$	$\mathcal{E}_M$	$\mathcal{E}_L$
	$(\delta)\ (\gamma'\ \delta'\ \epsilon')\ (\alpha\ \beta)$	$(\delta)\ (\epsilon\ \delta\ \gamma)\ (\beta\ \alpha)$	$(\delta^C)(\gamma'^C\delta'^C\epsilon'^C)\ (\alpha\ \beta)$	$(\delta^C)(\epsilon'^C\delta'^C\gamma'^C)\ (\beta\ \alpha)$
$(\forall x)$ $(1\ 0\ 0)$	$\boxed{(\forall x)\ (\underline{\underline{s}}\ x)}$ $(1)\ (1\ 0\ 0)\ (1\ 0)$	$(\Phi x)\ (\neg\underline{\underline{s}}\ x)$ $(1)\ (0\ 0\ 1)\ (0\ 1)$	$\neg(\Lambda x)\ (\underline{\underline{s}}\ x)$ $(0)\ (0\ 1\ 1)\ (1\ 0)$	$\neg(\exists x)\ (\neg\underline{\underline{s}}\ x)$ $(0)\ (1\ 1\ 0)\ (0\ 1)$
(Φx) $(0\ 0\ 1)$	$\neg(\forall x)\ (\neg\underline{\underline{s}}\ x)$ $(1)\ (1\ 0\ 0)\ (0\ 1)$	$\boxed{(\Phi x)\ (\underline{\underline{s}}\ x)}$ $(1)\ (0\ 0\ 1)\ (1\ 0)$	$\neg(\Lambda x)(\neg\underline{\underline{s}}\ x)$ $(0)\ (0\ 1\ 1)\ (0\ 1)$	$\neg(\exists x)\ (\underline{\underline{s}}\ x)$ $(0)\ (1\ 1\ 0)\ (1\ 0)$
(Λx) $(0\ 1\ 1)$	$\neg(\forall x)\ (\underline{\underline{s}}\ x)$ $(0)\ (1\ 0\ 0)\ (1\ 0)$	$\neg(\Phi x)\ (\neg\underline{\underline{s}}\ x)$ $(0)\ (0\ 0\ 1)\ (0\ 1)$	$\boxed{(\Lambda x)\ (\underline{\underline{s}}\ x)}$ $(1)\ (0\ 1\ 1)\ (1\ 0)$	$(\exists x)\ (\neg\underline{\underline{s}}\ x)$ $(1)\ (1\ 1\ 0)\ (0\ 1)$
$(\exists x)$ $(1\ 1\ 0)$	$\neg(\forall x)\ (\neg\underline{\underline{s}}\ x)$ $(0)\ (1\ 0\ 0)\ (0\ 1)$	$\neg(\Phi x)\ (\underline{\underline{s}}\ x)$ $(0)\ (0\ 0\ 1)\ (1\ 0)$	$(\Lambda x)\ (\neg\underline{\underline{s}}\ x)$ $(1)\ (0\ 1\ 1)\ (0\ 1)$	$\boxed{(\exists x)\ (\underline{\underline{s}}\ x)}$ $(1)\ (1\ 1\ 0)\ (1\ 0)$

"canonical" form of the state, representable by just one three-element Boolean vector ($\gamma\ \delta\ \epsilon$) of BA-3. The primes on ($\gamma'\ \delta'\ \epsilon'$) which occurs in the standard form have been removed while expressing the QPL term in the canonical form.

The four equivalence operators $\mathcal{E}_E$, $\mathcal{E}_L$, $\mathcal{E}_M$, $\mathcal{E}_N$, interconvert the standard forms that are equivalent into one another. They form a group isomorphic to the well-known "Four group", with the following properties:

$$\mathcal{E}_E^2 = \mathcal{E}_L^2 = \mathcal{E}_M^2 = \mathcal{E}_N^2 = \mathcal{E}_E \ ; \qquad (19a)$$

$$\mathcal{E}_L\ \mathcal{E}_M = \mathcal{E}_M\ \mathcal{E}_L = \mathcal{E}_N \ ; \quad \mathcal{E}_M\ \mathcal{E}_N = \mathcal{E}_N\ \mathcal{E}_M = \mathcal{E}_L \ ;$$
$$\mathcal{E}_N\ \mathcal{E}_L = \mathcal{E}_L\ \mathcal{E}_N = \mathcal{E}_M \qquad (19b)$$

In fact the four canonical states "for all" ($\forall$), "for none" (Φ), "not for all" (Λ) and "there exists" ($\exists$), are themselves related by QPL operators $\mathbb{E}$, $\mathbb{N}$, $\mathbb{M}$, $\mathbb{L}$, which are shown in Column 1 of Table 3. If now the above four states represented by canonical vectors in Column 2 of Table 4 are added and multiplied by Boolean operators $\oplus$ and $\otimes$ we get four more states. The names of these, as well as the new symbols coined for them, are shown in Fig. 1

Fig.1. Schematic representation of the 8 possible states in EQPL.

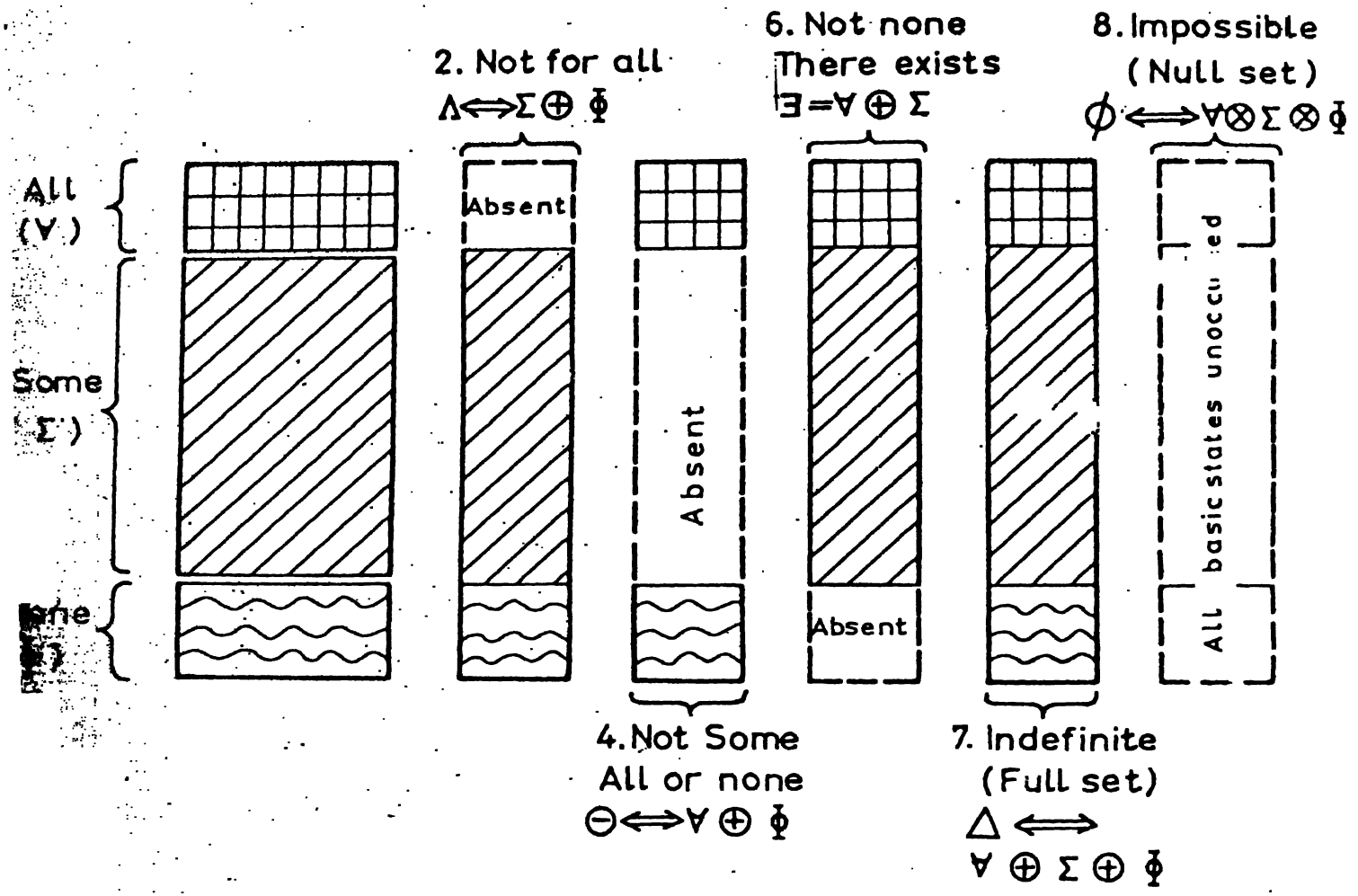

Fig.1. Schematic representation of the 8 possible states in EQPL

They are listed in Table 5 as the Boolean vectors comprising the representation of the 8 states of EPL (EPL standing for "Extended" Quantified Predicate Logic). These have been given the symbols q(1) to q(8) in that table, and the states into which each one goes, when operated by the EPL operators $\mathbb{E}, \mathbb{N}, \mathbb{M}, \mathbb{L}$, are also shown therein. In fact Table 5 is a complete truth table for these operators.

Table 5. Boolean vectors for the 8 states of EPL and their interconversions.

The four new states of EPL that have been thus obtained have the following properties. The most interesting is the new basic state Σ (for some), in addition to the two standard ones $\forall$ (for all) and Φ (for none). The state Σ (q(8)) means that only some exist, but not all or none. If we take the complement of "some", we get "all or none" (q(4)) indicated by the symbol Θ. Finally, we have the indefinite state (q(7) or Δ) which is obtained by adding all the three basic states $\langle \forall \rangle$, $\langle \Sigma \rangle$ and $\langle \Phi \rangle$, and a statement in this indefinite state (Δ x) ($\underline{s}$ x) has absolutely no logical information content for the term denoted by $\underline{s}$ x . However, anticipating the discussion in the next section, if the vidya operator ($\otimes$) is applied between this vector (1 1 1)

Table 5. Boolean vectors for the 8 states of QPL[+]

Sl.No. of state	Name of quantifier	Boolean vector ($\gamma\ \delta\ \epsilon$)	Symbol of state when operated by			
			$\mathfrak{E}$	$\mathfrak{N}$	$\mathfrak{M}$	$\mathfrak{L}$
q(1)	For all	(1 0 0)	$\forall$	Φ	Λ	$\exists$
q(2)	Not for all	(0 1 1)	Λ	$\exists$	$\forall$	Φ
q(3)	For some	(0 1 0)	Σ	Σ	Θ	Θ
q(4)	All or none	(1 0 1)	Θ	Θ	Σ	Σ
q(5)	For none	(0 0 1)	Φ	$\forall$	$\exists$	Λ
q(6)	There exists	(1 1 0)	$\exists$	Λ	Φ	$\forall$
q(7)	Indefinite	(1 1 1)	Δ	Δ	ϕ	ϕ
q(8)	Impossible	(0 0 0)	ϕ	ϕ	Δ	Δ

[+]Each of the four pairs consists of a set of two mutually complementary states — e.g. $\forall^c = \Lambda$, $\Sigma^c = \Theta$, $\Phi^c = \exists$, $\Delta^c = \phi$.

and one of the other seven states ($\gamma\ \delta\ \epsilon$), then the other state ($\gamma\ \delta\ \epsilon$) will be the output. Similarly, the "impossible" state $q(8)$ ($\emptyset$) is obtained by taking the intersection of all the three basic states $\forall$, Σ and Φ. Since they are mutually non-overlapping, their intersection will be the null set $\emptyset$, corresponding to the "impossible" state in logic and denoted by the Boolean vector (0 0 0) of EPL.

Before considering the effects of 3X3 matrix operators and the Boolean symbolic operators $\oplus$ and $\otimes$ on the eight BA-3 vectors representing (in the canonical form) the 8 states of EPL, we shall classify the 64 possible quantified terms in the standard notation, including the 16 of Table 5, which can occur in EPL. Thus,

(i) Quantifier is one of $\forall$, Φ, Λ, $\exists$ of QPL and $\underline{s}$ = T or F, sign = 0 or 1. These 16 were considered in Table 3, and lead only to 4 states.

(ii) Quantifier is one of the four new states of EPL, and $\underline{s}$ = T or F, sign = 0 or 1. These also lead only to four standard states (Σ x) ($\underline{s}$ x), (Θ x) ($\underline{s}$ x), (Δ x) ($\underline{s}$ x) and ($\emptyset$ x) ($\underline{s}$ x), each of which produces a set of ~~four~~ two equivalent standard forms, by the application of the modifiers $\mathcal{E}_E$, $\mathcal{E}_N$, $\mathcal{E}_M$, $\mathcal{E}_L$

(iii) either
(ϕ) Quantifier is any one of eight, sign ~~eight~~ "yes" or "no" (0 or 1) but $\underline{\underline{s}} = D$. All sixteen of these lead to the same canonical state $\Delta\,(\equiv(\Delta\,x)\,(\underline{\underline{s}}\,x))$.

(iv)
~~(d)~~ Quantifier is any one of eight, sign either "yes" or "no" (0 or 1), but $\underline{\underline{s}} = X$. Again all sixteen lead to the same canonical state $\phi\,(\equiv(\phi\,x)\,(\underline{\underline{s}}\,x))$.

Just as with the set of states (i), the properties of those in ~~(b)~~ (ii), ~~(c)~~ (iii), ~~(d)~~ (iv) above have been formulated by us from an examination of the logical contents, and equivalences, of the relevant standard forms. The effect of $\underline{\underline{s}} = D$ can be explained by saying that if the statement $\underline{\underline{s}}$ has a doubtful state and can give no information, then it converts itself automatically into the universally doubtful quantified state Δ Similarly $\underline{\underline{s}} = X$ leads straightaway to the impossible quantified state ϕ. Further details are reserved for a more extensive presentation elsewhere.

(d) Canonical states of EPL and their use with connectives

Since the eight canonical states, isomorphic to the 8 states of BA-3, cover all the standard forms of terms in EPL, we shall only consider connective operators (unary and

binary) which interconnect these canonical states. While doing this, we shall indicate how all the well-known connectives of quantified predicate logic are covered and their properties (as envisaged in standard presentationson the subject) are all incorporated in our formulation. We shall first indicate how a standard form $\mathcal{A}'$ is converted to its canonical form $\mathcal{A}$ and how a unary connective $\mathcal{Z}$ is applied to it to obtain the canonical form $\mathcal{b}$ of the resulting term, which can then be modified into the required standard form.

This is illustrated by an example in Table 6 (a, b, c). The problem to be solved can be stated in words as follows:

We are given that "For all x, $\underline{a}$x is true implies that there exists a y such that $\underline{b}$ y is true" (Step (b)). For this relation, the input is "There does not exist any $\underline{a}$ x that is false" (Step (a)), and we are asked to find out, given the quantifier state ($\forall$ y) of the output, what is the nature of $\underline{b}$ y, and the sign of the quantifier (Step (c)).

The three steps involved are indicated schematically in Table 6, the most important of which is the representation

Table 6. Example of a QPL sentence in an argument implemented via canonical terms and connectives.

Table 6. Example of a QPL sentence in an argument implemented via canonical terms and connectives

Description of sub-step	Logical content and Boolean algebraic representation
(a) Input canonized	$\neg(\exists x)\ (\neg \underline{a}\ x) \overset{C}{\Longrightarrow} (\forall x)\ (\underline{a}\ x)$ $(0)\ (1\ 1\ 0)\ (0\ 1) \overset{C}{\Longrightarrow} (1\ 0\ 0)$ (Standard form) (Canonizer) (Canonical form)
(b) Canonical connective applied	$\forall(x) \Longrightarrow \exists(y)$ $(1\ 0\ 0)\ \ \mathbb{I}(1, 6) \rightarrow (1\ 1\ 0)$; $\mathbb{I}(1, 6) = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$ (Canonical) (Connective) (Canonical)
(c) Output standardized	$\exists(y)\ (\underline{b}\ y) \overset{S}{\Longrightarrow} \neg(\forall y)\ (\neg \underline{b}\ y)$ $(1\ 1\ 0) \overset{S}{\Longrightarrow} (0)\ (1\ 0\ 0)\ (0\ 1)$ (Canonical form) (Standardized) (Standard form)

of the connective involved, namely "implies" in Step b. Anticipating the form of this (namely one of the sixty four 3X3 matrices for "implies" — see Section 6), we state that it is $\mathbb{I}(1, 6)$ in the present case, the indices 1 and 6 standing for $\forall = q(1)$ and $\exists = q(6)$, which are connected by it . Since this BA-3 matrix requires that both the input and output vectors are in BA-3, i.e. the canonical form, Step (a) applies the "canonizer" first to convert the input from the standard form to the canonical form. The algorithm for the canonizer is given in Part A of Table 6 in Section 6(b)(ii). Similarly, when the output comes out in the canonical form, the "standardizer" of Step (c) converts it into the required standard form. The algorithm for the standardizer is given later in Table 6, Part B.

Although this example does not involve all the intricacies related to problems of this kind, it gives the essence of our procedure, and we obtain the required result in Step (c) — namely "Not for all y is the statement b y false".

The operator $\mathbb{I}(1, 6)$ is a 3X3 Boolean matrix. Similarly, other connectives such as "and", "or", "nand" etc., of EPL are also matrix operators. These are discussed in Section 6(c)(iii), where their nature is derived physically by inspecting

their expected logical nature. In doing this, we apply the procedure normally adopted in theoretical physics — namely of examining the properties of the connective as it is considered in standard QPL, and then giving them a mathematical interpretation using EA-3 for EPL (which includes QPL). In this sense, our method of approach is similar to the use of algebraic formulae and equations in Cartesian analytical geometry, for solving problems in pure geometry. On the other hand, standard treatments of logic via theorems follow the method of Euclidean geometry in deriving proofs with existence conditions rather than giving a technique for working out problems. We believe that our method will solve problems very readily as will be shown in Section 7.

6. Non-matrix and matrix connectives in EPL

(a) Unary connectives $\mathbb{E}$, $\mathbb{N}$, $\mathbb{M}$, $\mathbb{L}$ for affirmation and negation

As shown in Table $\overset{4}{\beta}$, Section 5(c), these operators permute the four states $\forall$, $\overline{\Phi}$, Λ, $\exists$, among themselves, and similarly permute the two states Σ and Θ between themselves and Δ and $\emptyset$ within the pair. The algebraic equations that define these transformations, for the operator in $\mathbb{Q}\,\mathbb{Z} = \mathbb{b}$

(for $\mathbb{E}$ = affirmation, $\mathbb{N}$ = negation, $\mathbb{M}$ = complementation and $\mathbb{L}$ = ellation:), are

$$\mathbb{Z} = \mathbb{E}: \quad a_\gamma = b_\gamma, \quad a_\zeta = b_\zeta, \quad a_\epsilon = b_\epsilon \tag{20a}$$

$$\mathbb{Z} = \mathbb{E}_\lambda^{\mathbb{N}}: \quad a_\gamma = b_\epsilon, \quad a_\zeta = b_\zeta, \quad a_\epsilon = b_\gamma \tag{20b}$$

$$\mathbb{Z} = \mathbb{E}_\lambda^{\mathbb{M}}: \quad a_\gamma^c = b_\gamma, \quad a_\zeta^c = b_\zeta, \quad a_\epsilon^c = b_\epsilon \tag{20c}$$

$$\mathbb{Z} = \mathbb{E}_\lambda^{\mathbb{L}}: \quad a_\gamma^c = b_\epsilon, \quad a_\delta^c = b_\zeta, \quad a_\epsilon^c = b_\gamma \tag{20d}$$

It is readily verified that $\mathbb{N}^2 = \mathbb{M}^2 = \mathbb{L}^2 = \mathbb{E}$, so that all three have the nature of negating a term to which they are applied, but in three different ways.

(b) Binary connectives $\mathbb{E}$ and $\mathfrak{G}_n$.

The unary "affirmation" operator $\mathbb{E}$ is also the binary "equivalence" operator, for which the matrix form

$$|E| = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{21a}$$

is the best representation for practical use. Thus, if

$$(a \Longleftrightarrow b) = a\,\mathbb{E}\,b = (a\,|\,E\,|\,b) = (1 \quad 0) = T \tag{21b}$$

then a and b have the same 3-vector canonical form. However

just as in SNS, this operator does not have the property of giving F if $a \Longleftrightarrow b$. For this purpose, we require the "agreement" operator G, similar to the SNS $\underset{\sim}{G}$. (see Ref.[5]). We also define this operator G in EPL, similar to SNS, by the equations

$$(a\ G\ b) \Longleftrightarrow a_\gamma = b_\gamma,\quad a_\delta = b_\delta,\quad a_\epsilon = b_\epsilon \qquad (22)$$

The binary operator G gives T if the three components of the two 3-vectors are all alike, and F otherwise. It is useful for designing the canonizer and the standardizer discussed in the next section. For lack of space, we shall not give the Boolean algebraic expression for $(a \mid G \mid b) = \underset{\sim}{c}$.

(c) Canonizer and Standardizer

We utilize the formulae in Tables 7(a) and 7(b) for this purpose. Taking Table 7(a), it can be verified that the application of the canonizer Z gives

$$q' Z = q \qquad (23)$$

where $q' = (q'_\gamma\ q'_\delta\ q'_\epsilon) = (\gamma'\ \delta'\ \epsilon')$ of the standard form $(\delta)\ (\gamma'\ \delta'\ \epsilon')\ \alpha\ \beta)$, and $q = (\gamma\ \delta\ \epsilon)$. The nature of Z is as in column 3 of Table 6(a).

Table 7. Algorithmic Table for the Canonizer and Standardizer

Table 7. Algorithmic Table for the Canonizer and Standardizer

(a) Canonizer $\mathcal{Q}' \mathbb{Z} = \mathcal{Q}$

Sign $\hat{S}$	State of sentence $\underline{s}$ $(\alpha\ \beta)$	Canonizer $\mathbb{Z}$
1	T (1 0)	$\mathbb{E}$
1	F (0 1)	$\mathbb{N}$
0	T (1 0)	$\mathbb{M}$
0	F (0 1)	$\mathbb{L}$
~~Any~~	D (1 1)	$\mathbb{D}^+$, $\mathcal{Q} = \Delta$
Any	X (0 0)	$\mathbb{X}^+$, $\mathcal{Q} = \phi$

(b) Standardizer, yielding $\hat{S}$ and $(\alpha\ \beta)$, given $\mathcal{Q}$ and $\mathcal{Q}'$

Value of j for $E_j = T$	Standardized state		
	$(\hat{S})$	$(\mathcal{Q}'\ \mathcal{S}'\ \mathcal{E}')$	$(\underline{\alpha}\ \beta)$
1	1	$\mathcal{Q}\mathbb{E}$	T(1 0)
2	1	$\mathcal{Q}\mathbb{N}$	F(0 1)
3	0	$\mathcal{Q}\mathbb{M}$	T(1 0)
4	0	$\mathcal{Q}\mathbb{L}$	F(0 1)
None	1	$\mathcal{Q} \underset{\approx}{\vee} \mathcal{Q}' = \mathcal{Q}''$ $\mathcal{Q}'' \mathbb{E} \mathcal{Q} = \underline{s}\ (\alpha\ \beta)$	$\hat{S}$

+These are defined in subsection (vi), but we can straightaway write $\mathcal{Q} = \Delta = (1\ 1\ 1)$ in the former case, and $\mathcal{Q} = \phi = (0\ 0\ 0)$ in the latter.

For the standardizer, we use the information taken in for the canonizer in the reverse direction. We suppose that the canonical state $\mathcal{Q}\gamma = (\gamma\ \delta\ \epsilon)$ is given, and we require $(\hat{S})$ and $(\alpha\ \beta)$, given $\mathcal{Q}\gamma' = (\gamma'\ \delta'\ \epsilon')$ of the standard form $(\hat{S})\ (\gamma'\ \delta'\ \epsilon')\ (\alpha\ \beta)$. This is done as follows.

(i) Calculate $\mathcal{N}_1$, $\mathcal{N}_2$, $\mathcal{N}_3$, $\mathcal{N}_4$, equal to $\mathcal{Q}\gamma\, \mathcal{Z}$ for $\mathcal{Z} = \mathbb{E}, \mathbb{N}, \mathbb{M}, \mathbb{L}$ respectively, and find out the SNS state of $(\mathcal{N}_j \mid G \mid q') = g_j$.

(ii) If g_j is T, for some $j = 1, 2, 3$ or 4, then the standardized state is given by the six elements, in the row corresponding to j, in Table 6(b).

(iii) If all g_j are F, $\hat{S}$ can be taken to be 1, and we calculate $\mathcal{Q}\gamma \underset{\approx}{V}\, \mathcal{Q}\gamma' = \mathcal{Q}\gamma''$ and then the SNS state of the relation $(\mathcal{Q}\gamma'' \mid E \mid q)$, (one of T, F, D, X) gives the state of s. These are summarized in Table 6(b).

The proofs of these are reserved for a detailed paper.

(d) Boolean operator connectives $\underset{\approx}{\overset{\wedge}{\vee}}$ and $\underset{\approx}{\overset{\vee}{\vee}}$ in BA-3

We have already seen that these two operators $\underset{\approx}{U}$ and $\underset{\approx}{V}$ in logic, respectively correspond to the Boolean "sum" $(\oplus)$

and the Boolean "product" ($\otimes$) in Boolean algebra. They have been defined already for n-vectors and used for SNS in [1] , corresponding to BA-2. Similarly, the operator $\vee$ used in $\alpha' \vee \alpha''$ in BA-3, brings out the state that is common to two state-vectors α' and α''. For example, if $\alpha' = \forall = (1\ 0\ 0)$, and $\alpha'' = \exists = (1\ 1\ 0)$, then $\alpha' \vee \alpha''$ is $(1\ 0\ 0) \otimes (1\ 1\ 0) = (1\ 0\ 0)$, i.e. "for all". (Note the analogy to the concept of "intersection" in set theory. However, the connective "and" in QPL has other interpretations, representable by 64 possible matrices $A(i, j)$, $i, j = 1$ to 8, (as shown in Section 6(f) below) in EPL).

On the other hand, if the logical operation has the property of taking as true the information provided by either one of the two sources, (as with rumour), then we must employ the connective-operator $\cup$. (Note the connection, in this case, with "union" in set theory. Here again "or" in QPL is described in full, only by a set of 64 $O(i, j)$ operators see (f) below).

(e) Singular matrix connectives

As we have already seen, the input and output vectors in EPL are all canonical 3-vectors of the type $\alpha \equiv (a_\gamma\ a_\delta\ a_\epsilon)$

and $/\!b = (b_\gamma\ b_\delta\ b_\epsilon)$, so that a general matrix connective between them is representable by a 3X3 Boolean matrix $|Z|$. Any matrix connective $\mathcal{Z}$ in EPL is thus representable by $|Z|$, which is a sum of matrices ~~$|S(\lambda,\mu)|$~~ as

$$|Z| = \sum_{k=1}^{K} |S_{\lambda_k, \mu_k}|, \qquad K \leq 9 \tag{24}$$

The matrix ~~$S(\lambda,\mu)$~~ $|S_{\lambda\mu}|$ has a component $S_{\lambda\mu} = 1$ (λ, μ = one of γ, δ, ϵ), and 0 otherwise, and may be called the "singular matrix" ~~$S(\lambda,\mu)$~~ $|S_{\lambda\mu}|$, and a general 3X3 Boolean matrix is a sum of at most nine such singular matrices. Thus, the "and" relation between $(a_\gamma\ 0\ 0)$ and $(0\ 0\ b_\epsilon)$ is

$$(a_\gamma\ |\ \text{~~$S(\gamma,\epsilon)$~~ } |\ a_\epsilon) = (c_\alpha\ c_\beta) \tag{25}$$

$|S_{\gamma\epsilon}|$

and this will give $\underline{c} = T$ only for $\mathcal{a} = \forall$ and $/\!b = \bar{\phi}$ and $\underline{c} = F$, for all the other eight out of the nine possible combinations of the basic states.

Because of this, the result of any unary relation $\langle a\,|\,Z\,| = \langle b|$ or any binary relation $\langle a\,|\,Z\,|\,b\rangle = \underline{c}$ is a Boolean direct sum of the application of 9 or less singular matrices. However, we shall discuss below particular 3X3 matrices, since they have a direct logical interpretation in EPL.

(f) Sixty four operators each of types $/A$ and O and their relation to $\mathbb{I}$ and $\mathbb{J}$.

In logic, one often gets a relation like $\forall(x)\ \&\ \exists(y) = \underline{c}$. An examination of the relational matrix for the connective "and" in this shows that if the "and" is between a $q(i)$ and a $q(j)$, then the matrix $/A_{\lambda\mu}$ has non-zero elements for those λ for which the elements of $q(i)$ are non-zero and for those μ for which the elements of $q(j)$ are non-zero. Considering our case, $\forall$ corresponds to $i = 1$, and only $q_\gamma(1)$ is non-zero and $\exists$ corresponds to $j = 6$ (of Table 5), with $q_\gamma(6)$, $q_\delta(6)$ non-zero. Then the corresponding matrix for $/A(1, 6)$ has only $A_{\gamma\gamma}$, $A_{\gamma\delta}$ non-zero out of its 9 components. Thus,

$$|A(1, 6)| = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \text{for } (\forall\ \&\ \exists) \tag{26}$$

In the same way 64 $/A(i, j)$'s can be formulated, for the 64 "and" relations, $q(i)\ /A(i, j)\ q(j)$ with $i, j = 1$ to 8 (for specific examples, see Section 7). The corresponding matrix $|A(i, j)|$ is, as in (26), the "outer product" of $|q(i)\rangle$ and $\langle q(j)|$ via the Boolean product operator $\otimes$ of BA-1, giving

$$|A(i, j)| = |q(i)\rangle \otimes \langle q(j)| \tag{27}$$

Table 8(a) illustrates the rule for the outer product. Similarly, the EPL "or", illustrated by $\mathbb{O}(1, 6)$ in Table 8(b), has for its matrix, the Boolean "outer sum" of $q(1)$ and $q(6)$. Hence, in general,

$$|\overline{0\ (i,\ j)}| = |q(i)\rangle \oplus \langle q(j)| \qquad (28)$$

[Proofs of (27) and (28) are omitted for lack of space.]

Table 8. Generation of $|A(1, 6)|$ and $|0(1, 6)|$ as the outer product and sum of $\langle q(1)|$ and $\langle q(6)|$

Using just the definitions (27) and (28) for $/\!\!A(i, j)$ and $\mathbb{O}(i, j)$, all the interrelations between "and", "or", "if" and "only if" are derivable, if we take over the definition of the complement $|Z^c|$ of $|Z|$ from the general theory of Section 2. The series of equations from (29) to (32) all follow purely from 3X3 Boolean matrix algebra, using the above correspondence with connective operators $/\!\!A$ and $\mathbb{O}$ of EPL, and by taking over the inter-relations between $\underset{\sim}{A}$, $\underset{\sim}{O}$, $\underset{\sim}{I}$, $\underset{\sim}{J}$ of SNS (see [1]).

We shall use the notation $q(i^c)$ also for $q^c(i)$, in which the relation between i and i^c is as in (29), if the serial numbers in Table 4 are used for $q(i)$ and $q(j)$ in (27)

Table 8. Generation of $|A(1, 6)|$ and $|O(1, 6)|$ as the outer product and sum of $\langle q(1)|$ and $\langle q(6)|$.

(a) $|A(1, 6)| = |q(1)\rangle \otimes \langle q(6)|$

q(1) \ q(6)	1	1	0
1	1	1	0
0	0	0	0
0	0	0	0

(b) $|O(1, 6)| = |q(1)\rangle \oplus \langle q(6)|$

q(1) \ q(6)	1	1	0
1	1	1	1
0	1	1	0
0	1	1	0

and (28),

$$i^c = i + 1, \quad j^c = j + 1, \quad \text{if } i \text{ and } j \text{ are odd}$$
$$i^c = i - 1, \quad j^c = j - 1, \quad \text{if } i \text{ and } j \text{ are even} \tag{29}$$

Then, the eight binary connective relations $\mathbb{A}$, $\mathbb{A}^c$, $\mathbb{O}$, $\mathbb{O}^c$, $\mathbb{I}$, $\mathbb{I}^c$, $\mathbb{J}$, $\mathbb{J}^c$ of classical logic have the interrelations given in (30 to 32) (not all are listed, but only the more essential ones). Thus,

$$\mathbb{A}(i, j) \equiv \mathbb{O}^c(i^c, j^c) \quad \text{(First de Morgan relation)} \tag{30a}$$

$$\mathbb{A}^c(i^c, j^c) \equiv \mathbb{O}(i, j) \quad \text{(Second de Morgan relation)} \tag{30b}$$

For the implications $\mathbb{I}(i, j)$ ("if", in the forward direction) and $\mathbb{J}(i, j)$ ("only if" in the forward direction), we have

$$\mathbb{I}(i, j) \equiv \mathbb{O}(i^c, j) \equiv \mathbb{A}^c(i, j^c) \tag{31a}$$

$$\mathbb{J}(i, j) \equiv \mathbb{O}(j^c, i) \equiv \mathbb{A}^c(j, i^c) \tag{31b}$$

$$\mathbb{I}(i, j) \equiv \mathbb{J}(j, i) \quad \text{(Contrapositive form)} \tag{31c}$$

Similarly, for the denials of the relations $\mathbb{I}$ and $\mathbb{J}$, we obtain Eqns (32 a, b).

$$\mathbb{I}^c(i, j) \equiv \mathbb{O}^c(i^c, j) \equiv \mathbb{A}(i, j^c) \tag{32a}$$

$$\mathbb{J}^c(i, j) \equiv \mathbb{O}^c(j^c, i) \equiv \mathbb{A}(j, i^c) \tag{32b}$$

Two of the $\mathbb{A}$'s require special mention, namely $\mathbb{D} = \mathbb{A}(7, 7)$ and $\mathbb{X} = \mathbb{A}(8, 8)$. $\mathbb{D}$ has the property of converting any vector q(i) into q(7) = (1 1 1) by the unary operation $\langle q(i) \mid D \mid$, while $\mathbb{X}$ does the opposite, namely converting all vectors q(i) into q(8) = (0 0 0) by the formula $\langle q(i) \mid X \mid$. These matrices have been used in Table 7.

In addition to these, we must mention the matrix representations of $\mathbb{E}$ and $\mathbb{N}$, which are used quite often.

$$\overline{\mathrm{E}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \mathrm{N} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \tag{33}$$

Thus, out of the 2^9(= 512) possible 3X3 Boolean matrices, only 130 are used for the connectives of EPL to serve as representations of commonly utilized logical relations. The others could be used for rare occasions, via the singular matrix sum representation for any 3X3 Boolean matrix. Some of them have good logical sense, e.g.

$$\mid \mathrm{R} \mid = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{34}$$

makes $\mathbb{b}$ always $\forall$ in $\mathbb{a}\,\mathbb{R} = \mathbb{b}$, irrespective of the state of $\mathbb{a}$; but we shall not describe any of these.

7. Application of Vector-matrix Algebra to EPL

In this last section, we have considered the algebra of the logical connectives of EPL. These are however, applicable only to the canonical form of QPL terms. We shall now consider the use of these matrices for unary and binary relations of EPL, but with only one variable. The extensions to more variables, and to the cases where the sentence $\underline{s}$ itself contains more than one term connected by logical relations, can be made, but they are not discussed in this paper.

(a) Binary relations: It has not been recognized so far, that the 3X3 matrix that represents a particular relation (e.g. "and") is not unique, but has 64 variations in the BA-3 representation — $/\!\!A(i, j)$, i, j = 1 to 8. Thus, taking $/\!\!A(1, 6)$ illustration (see Table 7), it has the necessary property that it will give

$$(a \mid A(1, 6) \mid b) = T \tag{35a}$$

only if

$$\begin{aligned} &\langle a \mid \in \langle q(1) \mid (= \forall) = (1\ \ 0\ \ 0) \quad \text{and} \\ \text{and}\quad &\langle b \mid \in \langle q(6) \mid (= \exists) = (1\ \ 1\ \ 0) \end{aligned} \tag{35b}$$

This agrees with our intuitive concept of the "and" relation and, for $a/\!\!A(1, 6)/\!\!b = \underline{c}$ we have for any input states of

a (= q(k)), and b (= q(ℓ)), the equations

$$\langle q(k)|\ A(1,\ 6)|\ q(\ell) \ = \ c_\alpha \tag{36a}$$

$$\langle q(k)|A^c(1,\ 6)|\ q(\ell) \ = \ c_\beta \tag{36b}$$

$$(c_\alpha \quad c_\beta) \tag{36c}$$

giving the SNS state of the relation $\underline{c}$.

The same process can be applied for $O(i,\ j)$ (and for $A^c(i,\ j)$ and $O^c(i,\ j)$ also). Taking e.g., $O(1,\ 6)$, we can verify from the matrix that

$$(a\,|\,O(1,\ 6)|\ b) \ = \ T \tag{37a}$$

only if
~~demands that~~

$$\begin{aligned} \langle a|\in\langle q(1)|(=\forall) \ &= \ (1\ \ 0\ \ 0) \\ \text{or} \quad \langle b|\in\langle q(6)|(=\exists) \ &= \ (1\ \ 1\ \ 0) \end{aligned} \tag{37b}$$

which again agrees with our ideas regarding the logical connective "or", as applied to QPL.

It is quite likely that binary relations of the type $\underline{c}$ & d, where one is an SNS term and the other is a QPL term can occur. In such cases, we use 2X3 matrices $A(T,\ j)$ or $A(F,\ j)$ defined exactly as in (27). In this, $\langle q(i)|$ becomes

one of the basic SNS 2-vectors T(= (1 0)) or F(= (0 1)) as required, while $\langle a(j)|$ is an EPL 3-vector. A similar procedure is adopted for $/\!A(i, T)$ and $/\!A(i, F)$. We shall not pursue this further, but an example is given in Section 7(c).

The reversal of a binary relation gives a unary relation as explained in Section 3, and therefore we shall not discuss binary reverse connectives, but only unary connectives.

(b) Unary connectives: The most important unary connective is implies ($\Longrightarrow$) $\equiv \mathrm{I}(i, j)$. The straightforward way of obtaining this matrix is by its equivalent form $/\!A^c(i, j^c)$. That this has the necessary logical properties is seen as follows. We know that the SNS "implies" (I) gives for $\underline{a}\,\underset{\sim}{I} = \underline{b}$ the consequences $a_T \longmapsto b_T$, $a_F \longmapsto b_D$. In the same way, if we take, for example, $a\,\mathrm{I}(1, 6) = |b$, then $(a = \forall) \longmapsto (|b = \exists|)$, and $(a = \neg\forall = \Lambda) \longmapsto (|b = \Delta)$. The matrix $|I(1, 6)| = |A^c(1, 5)|$ is readily seen to have these properties. It is also seen that the analog, in EPL, of the SNS ~~matrix relation~~ equivalence $(\langle a|\, I| = \langle b|) \Longleftrightarrow (\langle b|\, J| = a)$, where $I^t = J$, is (31c).

With these preliminaries, we shall work out a practical example to indicate how facile the matrix representation of EPL and SNS is for working out actual problems.

(c) The audience-concert-crowd problem

The problem given below employs unary and binary QPL connectives, an SNS to QPL connective, and also the canonizer and standardizer. The problem is first stated in words, then in our notation for logic, and finally in the vector-matrix formalism. The reversal of the steps is, however made completely in the matrix formalism, except for the last step of translating the result into the form required. It is obvious that all the steps are computerizable.

Problem

(i) If not all the audience seats are unoccupied, and some of the musicians are present, the concert will go on.

(ii) If the concert takes place, all windows will be opened, otherwise all windows are shut.

(iii) If some windows are open, the verandah will be partly or fully filled with people listening to the music.

(iv) There are no people found in the verandah. Prove that, if, in addition, all seats are occupied, no musicians have come.

We write the three steps of the problem in the standard notation of EPL in Table 5.9.

Table 5.9. EPL problem in standard notation

(α) Boolean-algebraic notation

The relevant equations are (38), (39), (40) and we explain them below.

Part A

$$(0\ \ 1)\ (0\ \ 0\ \ 1)\ (1\ \ 0) \xRightarrow{c} (1\ \ 1\ \ 0) = q(6) \text{ for } \underline{s} \qquad (38a)$$

$$(1\ \ 0)\ (1\ \ 1\ \ 0)\ (1\ \ 0) \xRightarrow{c} (1\ \ 1\ \ 0) = q(6) \text{ for } \underline{m} \qquad (38b)$$

$$(\exists\ s)\ \mathbb{A}(6, 6)\ (\exists\ m) = \underline{c}\ ; \quad |A(6, 6)| \equiv \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad (38c)$$

Part B

$$\underline{c}\ \mathbb{R} = \mathbb{W}, \qquad |R| = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad (39a)$$

(l.c.)

Verify:

$$(1\ \ 0) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = (1\ \ 0\ \ 0)\ ; \quad (0\ \ 1) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = (0\ \ 0\ \ 1) \qquad (39b)$$

Table 9. QFL problem in standard notation

	Symbols	Logical equations in standard form
A	Seats $\underline{s}$ x ; Musicians $\underline{m}$ y Concert $\underline{c}$	$\neg(\bar{\Phi}\, x)\ (\underline{s}\ x)\ \&\ (\exists\ y)\ (\underline{m}\ y) = \underline{c}$
B	Window $\underline{w}$ z	$\underline{c} \Longrightarrow (\forall\, z)\ (\underline{w}\ z),\quad \neg\underline{c} \Longrightarrow (\bar{\Phi}\, z)\ (\underline{w}\ z)$
C	People $\underline{p}$ u	$(\exists\, z)\ (\underline{w}\ z) \Longrightarrow (\exists\, u)\ (\underline{p}\ u)$ (Note: $(\exists\, u) \equiv (\forall\, u) \oplus (\leq u)$)

Part C

$$(\exists w)\ \mathbb{I}(6,\ 6) = (\exists p)\ ;\ |I(6,\ 6)| = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{pmatrix} \qquad (40a)$$

Verify:

$$(1\ \ 1\ \ 0)\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{pmatrix} = (1\ \ 1\ \ 0) \qquad (40b)$$

$$(1\ \ 1\ \ 0) \xRightarrow{S} (1)\ (1\ \ 1\ \ 0)\ (1\ \ 0) \qquad (40c)$$

We first canonize the inputs for Part A of Table 9 in (38 a, b), and then select the right $\mathbb{A}(i, j)$ to connect the canonical inputs to give $(c_\alpha\ \ c_\beta)$, as shown in (38c). Next, we formulate the SNS—QPL connective "imply" of Part B by a 2X3 matrix. For $\underline{c} = T(1\ \ 0)$, $\overset{w}{\underline{p}} = \forall = (1\ \ 0\ \ 0)$, and for $\underline{c} = F = (0\ \ 1)$, $\overset{w}{\underline{p}} = \Phi = (0\ \ 0\ \ 1)$. Hence the relational matrix $\mathbb{R}$ of (39a) is obtained for the relations in this Part B, and it is verified that it has the required properties in (39b).

Part C of Table 9 is straightforward, since it is a unary relation, and both input and output are already in the canonical form. The canonical equation for this, and the relevant matrix $\mathbb{I}(6, 6)$ are shown in (40 1a 9) and (9b). If necessary, the $(\exists \underline{p})$ can be standardized to $(\exists u)\ (\underline{p}\ u)$ as in (40c).

(β) Reversal of the steps in Boolean algebraic notation.

In reverse, the two inputs are:

(i) "No persons are in the verandah", which in canonical BA form, is

$$(\overline{\exists}\, p) \;=\; (0\ \ 0\ \ 1) \text{ for } \|p\,. \tag{41a}$$

and

(ii) "All seats are occupied", which in canonical BA form, is

$$(\forall s) \;=\; (1\ \ 0\ \ 0) \text{ for } \mathcal{S}\,. \tag{41b}$$

We shall simply reverse the canonical equations in (40), (39) and (38), and write them as (42c, b, a) respectively, in that order, to represent the reversals of Parts C, B, A of Table 8.9

$$\langle p \,|\, I^t\,(6,\,6)| \;=\; \langle w| \quad (3 \text{ vector}) \tag{42c}$$

$$\langle w \,|\, R^t| \;=\; \langle c| \quad (2\text{-vector}) \tag{42b}$$

and

$$\left.\begin{array}{l} \langle s|\, A| \;=\; \langle m| \quad (3\text{-vector}),\ \text{if } \underline{c} = T \\ \langle s|\, A^c| \;=\; \langle m| \quad (3\text{-vector}),\ \text{if } \underline{c} = F \end{array}\right\} \tag{42a}$$

Now $\langle p| \;=\; (0\ \ 0\ \ 1)$, so that $\langle p|\, I^t\,(6,\,6)|$ is

$$(0\ \ 0\ \ 1)\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix} \;=\; (0\ \ 0\ \ 1) \text{ for } \langle w| \tag{43}$$

Putting $\langle w| = (0\ \ 0\ \ 1)$ in (42b), we get

$$(0\ \ 0\ \ 1)\begin{vmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{vmatrix} = (0\ \ 1) \text{ for } \langle c| \qquad (44)$$

Since $\underline{c} = F$, we have the second equation in (42a), and hence

$$\langle s|\, A^c| = \langle m| \qquad (45a)$$

In this, by (41b), $\langle s| = \langle 1\ \ 0\ \ 0|$ in QPL, and taking the complement of $|A(6,\ 6)|$ in (38c) for $|A^c|$, we obtain

$$(1\ \ 0\ \ 0)\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix}(0\ \ 0\ \ 1) = \langle m| \qquad (45b)$$

Standardization of $\langle m| = (0\ \ 0\ \ 1)$ is straightforward, and $\mathfrak{M} = (\underline{\Phi}\ y)\ (\underline{m}\ y)$, i.e. "No musicians are present" (QED).

(d) Concluding remarks

Thus, we have effectively converted the axioms and rules of EPL into vector-matrix equations, associated with the usual logical functions (NOT, AND, OR, XOR (of BA-1)) available in a computer. As a matter of fact, just like MATLOG for SNS, it is not at all difficult to write a program in FORTRAN IV for all

that we have discussed in this paper. Our technique is therefore eminently practical and suitable for expanded application to more complicated formulae in SNS and QPL.

— On the purely theoretical side, the most interesting aspect is the introduction of the new basic state "some" (Σ), which is quite enigmatical for the common man. It was so for the Jaina philosophers in India in the B.C's, and they gave this indefinite state the name "avaktavya"(indescribable) [6] along with the simple words "true" and "false" for the two definite states (see [1]). Godel's demonstration [7] that any theory in PL, which is large enough, must contain theorems in this state (neither provable, nor disprovable) is therefore not an enigma for epistemology as it appears to be at first sight, but a necessary consequence of the structure of QPL, when extended into EPL. If the state Σ is needed for the completeness of QPL so as to be isomorphic to BA-3, there must be some statements in any system of logic isomorphic to BA-3, which possess the property of this Σ state — namely that of neither complete truth, nor complete falsity, both of which are unprovable. That this is true of some theorems in any theory making use of QPL is the beauty of Godel's theorm (see [4]) for a discussion of this).

Acknowledgements

The author wishes to thank Mr. T.A. Thanaraj and Mr. R.E.C. Johnson for checking many of his ideas by computer programs and logic circuits, and Professors M. Venkataraman, E.V. Krishnamurthy, D. Balasubramanian and Mr. Harishankar Ramachandran for numerous discussions. The work reported here was supported by an Extramural Grant from CSIR, India.

References and Notes

1. G.N. Ramachandran, Syad Nyaya System (SNS) — A New Formulation of Sentential Logic and its Isomorphism with Boolean Algebra of Genus 2, Current Science (Bangalore), 51, 625-36 (1982).

2. G. Birkhoff and S. MacLane, A Survey of Modern Algebra Fourth Edition (Macmillan Publishing Company) New York, 1977.

3. P. Suppes, Introduction to Logic, Van Nostrand Reinhold Company, New York, 1957.

4. R.R. Stoll, Set Theory and Logic, W.H. Freeman and Company, San Francisco, 1961.

5. G.N. Ramachandran and T.A. Thanaraj, Matrix Algebra for Sentential Logic and the FORTRAN program MATLOG, Matphil Reports No. 18, pp 1-64 (1981).

6. M. Hiriyanna, Outlines of Indian Philosophy, George, Allen and Unwin, Bombay, 1976, p. 164.

7. K. Godel, Monatsh Math. Physik, 193, pp 173-198 (1931)

EARLY EXPERIENCES WITH THE DYNAMICAL THEORY OF X-RAY DIFFRACTION

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Contribution to the Hildebrandt Festschrift
to be published in Zeitschrift fur Naturforschung.

This review summarizes some of the early studies on perfection of crystals, in relation to the dynamical theory of x-ray diffraction, which were carried out in the author's laboratories at Bangalore and Madras, during the 1940's, 50's, and early 60's. The Rayleigh theory of optical reflection from a stratified medium was shown to be identical in content with the Darwin theory for x-ray reflection from a perfect crystal. It was also shown to be identical in principle and leading to the same final equations as the Ewald-Laue-Zachariasen formulation for the "Bragg case". A consequence of the Borrmann effect, namely that sufficiently thick crystal plates can exhibit a sharp peak in transmission (as in reflection), was proved from theory for the conditions corresponding to its actual experimental observation made by Campbell in 1951, and even the shift between the settings for the two peaks was predicted from theory. The name "x-ray topograph" was coined by Prof. Raman, and used by the author, for the first time in 1944, for a photograph obtained by x-ray diffraction showing variations of degree of perfection over the surface of a crystal plate. The polarization method of measuring the degree of perfection (Δ) of a crystal was evolved in the early 50's by the author and Ramaseshan in Bangalore, and applied for measuring Δ in later years by K.S. Chandrasekharan in Madras. The fact that the integrated reflection of a perfect crystal can, under suitable conditions, exceed that of a mosaic crystal of the same size and shape, was both theoretically predicted and experimentally verified for calcite in the early 1960's in Madras.

1. Rayleigh formulation of the dynamical theory

The essential difference between the kinematical and the dynamical theory of x-ray diffraction is the following :

In the kinematical theory, the incident wave is supposed to go on unchanged in amplitude, and the reflected waves from the successive lattice planes in the crystal add up to give the total reflected beam. On the other hand, in the dynamical theory, the transmitted wave field interacts with the reflected wave field and there are multiple reflections of the electromagnetic waves forwards and backwards from the lattice planes in the crystal, and the resultant transmitted and reflected beams are obtained as a result of such multiple interactions. It is not recognized that the occurrence of such multiple reflections from stratifications, arising from repeated twinning at regular intervals, was observed by Stokes as early as 1885 in the field of optics and that the theory of "The Reflection of Light from a Regularly Stratified Medium" was given by Lord Rayleigh [1] in 1917, almost contemporaneous with the Darwin theory [2] of 1914 and the Ewald dynamical theory [3,4] of 1916 and 1917, regarding the corresponding phenomenon in x-rays. The optical phenomenon, known as "iridescence" is observed best in some crystals of multiply twinned potassium chlorate, and an example described by R.W. Wood was calculated to have some 700 alternations of refractive index, and a very high degree of regularity [1].

The Darwin theory for a non-absorbing crystal is given in great detail in their book on x-rays by Compton and Allison [5] (together with the extension made by Prins [6] to a crystal having absorption), but both these theories deal only with a crystal having an infinite number of reflecting [illegible]. On the other hand, Rayleigh's theory is valid for a finite [illegible] although he takes absorption to be [illegible]

R and T (the amplitudes of the finally reflected and transmitted beams), in terms of r and t, the reflection and transmission coefficients of a single stratification), which are, in general, complex numbers. He obtained for these the following two elegant formulae :

$$\frac{R}{\sinh n\beta} = \frac{T}{\sinh \alpha} = \frac{1}{\sinh (\alpha + n\beta)} \qquad (1)$$

where

$$\frac{r}{\sinh \beta} = \frac{t}{\sinh \alpha} = \frac{1}{\sinh (\alpha + \beta)} \qquad (2)$$

Neither Darwin, nor Rayleigh, seem to have been aware of each other's papers, although, as we shall show below, the two theories are absolutely identical in content. It was in 1942 that Prof. Sir C.V. Raman gave this problem to me, as the very first assignment when I joined him for research, after graduation. He showed me the beautiful recurrence relations, as given in (6.27) of Compton and Allison's book, which contain the essence of Darwin's theory and which have been solved for an infinite number of planes by Darwin after making an extra assumption (as became evident later — see below). He then showed me the above Eqs. (1) and (2) of Rayleigh, and asked me to derive these for a finite number of planes, using Darwin's recurrence relations, which are unquestionably correct. I am mentioning these details because it indicates how very often methods of approach adopted in one field are not noticed by persons working in other fields. Professor Raman was catholic in his interests, and equally at home in optical and x-ray diffraction, and it was at his suggestion that many of the studies discussed below were made.

Very quickly, I was able to convert the Darwin recurrence relations into a series expansion leading to a polynomial $f_n(y)$, where

$$y = (1 + t^2 - r^2)/t \qquad (3)$$

However, the [illegible] series was not

lucky in discovering the correct book for this purpose — namely Joley, "Summation of Series" [7] in the library of the Indian Institute of Science, which contained exactly the series met with in my problem. The wonder was even larger, when the summed series led to results exactly of the same form as Eqs. (1) and (2), obtained by Rayleigh by an entirely different procedure.

We shall give this derivation below (see [8]) very briefly. Making a slight change from Compton and Allison's book, and referring the amplitudes of the reflected and the transmitted beams at the mid-points between lattice planes by R_s and T_s, we obtain

$$R_s = r\,T_s + t\,R_{s+1} \tag{4}$$

$$T_s = t\,T_{s-1} + r\,R_s \tag{5}$$

which leads to

$$R_1 = \left[y^{n-1} - \frac{(n-2)}{1!}\,y^{n-3} + \frac{(n-3)(n-4)}{2!}\,y^{n-5} - \ldots\right] R_n = f_n(y) R_n \tag{6}$$

giving

$$\frac{R_1}{R_n} = f_n(y) \tag{7a}$$

$$\frac{R_1}{T_{n+1}} = \frac{r}{t} f_n(y) \tag{7b}$$

and

$$\frac{T_1}{T_{n+1}} = \frac{1}{t} f_n(y) - f_{n-1}(y) \tag{7c}$$

The quantities R and T of (1) are then given by

$$R = \frac{R_1}{T_1}\,, \qquad T = \frac{T_{n+1}}{T_1} \tag{8}$$

so that everything hinges on obtaining the right expression for $f_n(y)$. This was done by putting

$$y = 2\cos\beta \tag{9a}$$

which gave

$$f_n(y) = \frac{\sinh n\beta}{\sinh \beta} \qquad (9b)$$

It was a very simple matter thereafter to obtain Eqs. (1) and (2), from (3), (7) and (8), using (9a) and (9b).

It may be mentioned that this problem was solved in about a week's time, and th main delay was in finding out the right way of summing up the series $f_n(y)$, which was done on a Sunday when Joley's book was hunted out in the library of the Institute.

2. Secondary Maxima from Rayleigh's formula

Experimental studies on the reflection of light from iridescent crystals of $KClO_3$ had been made in Prof. Raman's laboratory during the previous couple of years. Using a collimated beam and a pocket spectrograph, it was found that the spectrum of the reflected light contained a sharp maximum and that secondary maxima also occurred on either side, whose positions depended on the thickness of the crystal. Therefore, Raman suggested to me that I should work out the detailed intensity distribution in the reflected beam as a function of angle, assuming the wavelength to remain constant, for some suitable values of r and t. The results thus obtained for $R = |R_1/T_1|^2$ are shown in Fig.1, reproduced from my paper [8]. It will be seen that the primary maximum builds up in intensity with increasing n, and that its sharpness also increases. However, the reflection curve has a finite width even for very large n, as expected from the Darwin theory. (This point was, however, missed by Rayleigh). Also, for finite n, there are, in addition to the principal maximum, a series of subsidiary maxima, exactly as predicted by the Ewald-Laue theory of dynamic x-ray diffraction, for the analogous "Bragg Case" (See Zachariasen [11], Fig.3.12 and Pinsker [23], Fig.8.1). Even the possible asymmetry of the

that Raman and Krishnamurthy [9] photographed and measured these, and a typical example for $KClO_3$ is shown in Fig.2. The four "spectra" are for different settings of polarizer and analyzer. The features to be especially noted are — (1) The larger breadth of the central maximum in relation to the secondary maxima, and (2) the asymmetry of the latter in some cases.

3. Studies on the Dynamical Theory for X-rays

a) Comparison of the Ewald and Darwin Theories

In 1944, two years after the above-mentioned studies were made, I showed [10] how Rayleigh's formula for a finite set of n stratifications can be used to derive the Darwin Prins formula for $|R|^2$, by setting $n \longrightarrow \infty$ including both the real and imaginary components of the refractive index, as was done by Prins. Very soon thereafter, the beautiful book on "X-ray diffraction in crystals" by Zachariasen [11], which was published in 1945, reached us in India. I took this book as my bible for the subject of dynamical x-ray reflections, and I read it from cover to cover. As a result, it came to my notice that the Ewald theory, which Zachariasen had converted into a form suitable for practical applications, does not give exactly the same rocking curve as the Darwin theory for a perfect crystal of infinite thickness (see p.142 of Zachariasen's book). Obviously, both cannot be correct, and so I examined the origin of the difference, and was able to pinpoint it to an extra assumption made by Darwin, namely that $T_s = T_1 x^s$, in his derivation of $R = (R_1/T_1)$ and $T = \lim_{n \longrightarrow \infty} (T_{n+1}/T_1)$. While this is valid for the region of perfect (100%) reflection, it was found to be not true for the part of the rocking curve outside the central maximum. When the exact Rayleigh solution of Darwin's equations (for which no such assumption is made) is taken to the limit [illegible], and the intensity is averaged over the variations of intensity in the [illegible] fringes, (which become infinitely close [illegible]) the Darwin theory was [illegible] over complete [illegible] reproduc[illegible]

the two.

It is interesting that, in spite of the above result having been published in Acta Crystallographica in 1948, in a paper [12] forwarded from Prof. Bragg's laboratory in Cambridge, and the fact that Prof. Ewald himself approved the result (as mentioned in the paper), Pinsker [23] in 1978 quotes Fig. 3.16 of Zachariasen's book in p. 262 of his book, and states that the Ewald and Darwin theories give different results. I hope that the present review will rectify this false impression (See next section where the analytic forms of the results, derived using the Ewald-Laue formalism, and the Darwin-Rayleigh formalism are shown to be exactly identical).

b) Practical applications

Because of the familiarity with the dynamical theory of x-ray reflections, as given in Zachariasen's book, I worked out from it various formulae on mosaic and perfect absorbing crystals, that are of practical use to x-ray crystallographers while I was in Prof. Bragg's laboratory, although I was actually working on a different subject, namely diffuse reflection of x-rays, as my formal assignment. I then came to understand that Dr. P.B. Hirsch of the same laboratory, was also working on the same problem, and had obtained results quite similar to mine. Therefore, we two put our heads together, and wrote a paper [13] for Acta Cryst. in 1949 on the integrated intensities of perfect and mosaic crystals under various conditions (for the Bragg case). This paper is widely quoted in the later literature on this subject, for it contains many results of practical utility.

c) Studies on the Borrmann effect [14], [15]

After spending two years in Cambridge, I returned to Bangalore and started work on x-ray crystallography [illegible] was always [illegible]

theory, which appeared in Acta Cryst. [16], reached us. Immediately, the Zachariasen presentation and the Laue presentation of the Ewald dynamical theory were assembled together and the two formulae were written side by side by me, and shown to be absolutely identical, in content (as is to be expected). However, it was interesting to find that the Laue presentation could be written in such a manner as to lead to formulae which were symbolically of the same form as those derived from the Rayleigh theory. This was published in a paper in Proc. Indian Acad. Sci. in 1952 [17]. In this paper, the theory of both the "Laue" case (internal reflection) and the "Bragg" case (surface reflection) were examined. The principal result deduced was that a sharp maximum occurs in the transmitted beam in the 'Laue case', very close to the setting for the peak in the reflected beam, provided the crystal is absorbing and the crystal is sufficiently thick, so as to make $\mu t \gg 1$. Although Laue had shown that such an "anomalous transmission", which was first observed by Borrmann in 1941, could be explained by the dynamical theory, our attention was directed specifically towards a paper by Campbell [19] which appeared in 1951, and which described the occurrence of such a sharp maximum in the transmitted beam, observed using a double crystal spectrometer. We felt that if experiment shows such an effect and the kinematical theory does not at all predict anything like that, then the only refuge is the dynamical theory. Therefore along with Dr. Kartha, I examined the dynamical theory in great detail and we were able to prove that a sharp maxima almost as large as that in the reflected beam will be expected also in the transmitted beam. We gave this phenomenon the name x-ray "anti-reflection". Fig.3 shows the results calculated for the conditions of the specific experiment of Campbell's, taken from my paper which appeared in the Journal of Applied Physics [20], which showed also the shift of the crystal setting corresponding to the peak in the transmitted beam from that in the reflected beam.

mitted beam which is an absolutely fundamental condition required in the dynamical theory.

It is interesting that, quite independently, Hirsch [21] had also worked some of the results mentioned above. However, Hirsch did not consider the "Bragg case" in his paper [21], but we showed that, when the Ewald-Laue formulation of the dynamical theory is worked out carefully, expressions identical with the Rayleigh-Darwin formulation are obtained [17].

(d) Identity of the Ewald and Darwin formulations (for the "Bragg case" — surface reflection.)

We shall only draw attention to the relevant equations in Ref. [17]. The expressions for R and T for a general (asymmetric) surface reflection are :

$$R = \left|\frac{\chi_h}{\chi_{\bar{h}}}\right| \left|\frac{\sinh x}{\sinh (u+x)}\right|^2 \qquad (10)$$

$$T = \left|\exp\left\{-2\pi ikD\left(\frac{1}{\gamma_0} - \frac{\delta_1+\delta_2}{2}\right)\right|^2 \left|\frac{\sinh u}{\sinh (u+x)}\right|^2 \qquad (11)$$

(see Ref. [17] for the notation, which is an extension of that used by Laue. In fact, Ref. [17] contains also a glossary giving the corresponding symbols in the Laue and Zachariasen notations).

When the reflection is symmetric, $|\chi_h| = |\chi_{\bar{h}}|$ and (10) and (11) reduce to the expressions in (12) below:

$$R = \left|\frac{\sinh x}{\sinh (u+x)}\right|^2 ; \quad T = \left|\frac{\sinh u}{\sinh (u+x)}\right|^2 \qquad (12)$$

These may be compared to the following expressions which follow from Eqs. (1) and (12) for the Rayleigh-Darwin formulation of ours [8], namely :

$$R = \left|\frac{\sinh x}{\sinh (u+x)}\right|^2 ; \quad T = \left|\frac{\sinh u}{\sinh (u+x)}\right|^2 \qquad (13)$$

exactly the same as u and x in (12), indicating once again what was pointed out by me earlier, namely that the Ewald and Darwin approaches are absolutely identical in content, in spite of their apparently very different mathematical approaches.

(e) Integrated reflection and antireflection (transmission) in the Laue case

Although these were worked out partially by Hirsch [21], a more exact formulation than Laue's [16], avoiding certain approximations employed by him, was obtained by me in 1954 [18], and by Kato [22] the next year. Using these, elegant expressions for the integrated reflection and integrated transmission were worked out for a variety of cases. Although both my theory and Kato's are reviewed and presented by Pinsker ([23], Sections 4.6 and 4.7), since the formulae in my paper, which appeared in Proc. Indian Acad. Sci., are not available therein, I am quoting one or two here for ready reference, because of their elegance. Thus, for the Laue case of an absorbing crystal of finite thickness, using the Zachariasen parameters y, g and k, we can obtain the following formulae for R and T. (Shades of the Rayleigh-Darwin formulae (12) for the Bragg case may be seen in these):

$$R = \frac{e^{-P}(1+k^2)}{2|X|^2}\left[\cosh\left(\frac{P}{G}\,\mathrm{Im}\,X\right) - \cos\left(\frac{P}{G}\,\mathrm{Re}\,X\right)\right] \qquad (14)$$

$$T = \frac{e^{-P}(1+k^2)}{2|X|^2}\left[\cosh\left(\frac{P}{G}\,\mathrm{Im}X - 2\nu_r\right) + \cos\left(\frac{P}{G}\,\mathrm{Re}X - 2\nu_i\right)\right] \qquad (15)$$

where

$$X = \left[(y^2 - a^2G^2 + 1 - k^2) + 2i\,(k + ayG)\right]^{\frac{1}{2}} \qquad (16)$$

$$G = g/a \qquad (17a)$$

where a is the asymmetry factor

$$a = (1-b)/(1+b) \qquad (17b)$$

and

$$P = \frac{\pi D}{2}\left(\frac{1}{\gamma_0} + \frac{1}{\gamma_H}\right) \qquad (18)$$

and

(i) Symmetric reflection ($\gamma_0 = \gamma_h$)

The convenience of this elegant notation is seen from the following two expressions for the case of a symmetrical reflection (a = 0), with $k^2 \ll 1$, for the Integrated Reflection (R_y) and the Integrated Antireflection (T_y).

$$R_y = \frac{e^{-P}}{2}\left[\int_{-\pi/2}^{+\pi/2} \cosh\left(\frac{Pk\cos\theta}{G}\right)d\theta - \int_{-\infty}^{+\infty} \frac{\cos\left[P(\cosh t)/G\right]}{\cosh t}\,dt\right] \qquad (20)$$

$$T_y = \pi e^{-P}\left[\int_0^{Pk/G} dx' \int_0^{x'} I_0(x)\,dx - \tfrac{1}{2} I_0(j^P) + 1 \right.$$

$$\left. - \int_0^{P/G} I_0(x)\,dx\right] \qquad (21a)$$

where $$j^2 = a^2 + (k/G)^2 \qquad (21b)$$

and $I_0(x)$ and $I_1(x)$ are Bessel functions of imaginary argument, namely $J_0(ix)$ and $J_1(ix)$.

(ii) Thin crystal, weak reflection, large absorption and asymmetry

Under any of the conditions mentioned above (viz. P small, or G large), we obtain that

$$R_y = \frac{\pi}{2G} P e^{-P} \qquad (22)$$

and this expression is identical with the corresponding expression for a mosaic crystal. [See Ref. [18] for various intermediate cases.] This is the reason why extinction corrections become unimportant except for very strong reflections, if the crystal size is small enough.

The theoretical studies reported in this section formed the basis of a number of experimental investigations in our laboratory in Madras, on the degree of perfection of a crystal under a variety of conditions, and these are briefly reviewed in the next section.

4. Integrated Reflection and its Variation with Mosaicity

(a) X-ray topographs

It is well known that, normally, a perfect crystal [redacted] reflection (R

less than a mosaic crystal of the same material, and that R_y increases with increase of mosaicity, or occurrence of imperfections. A simple method of displaying the variations in the degree of perfection over the surface of a crystal plate was suggested to me by Professor Raman, in 1944. The Laue (internal) reflection from a set of (hkl) planes, approximately at right angles to the surface, is chosen, and a divergent beam of x-rays from a pinhole is obtained by having a defocussed source of finite area for the x-rays. (The defocussing was possible because we were working with a demountable x-ray tube, in which the distance from the filament to the target could be altered.) Then, an x-ray diffraction image of the whole crystal surface can be obtained on the film, kept at a suitable angle to the direct beam, corresponding to the Laue (white radiation) spot [24]. The name "x-ray topograph" was given to this image, since the variations of density in the image will correspond to the variations of R_y, and hence of the degree of imperfection, over different parts of the crystal. Two topographs of diamond (111) cleavage planes are shown in Fig.4, taken from Refs. [24 , 25]. There is a central region of larger intensity in the triangular x-ray topograph (Fig.3(b)) of D 180 (Type I), which corresponds to a similar central region of increased blue luminescence of Fig.4(a). On the other hand, the diamond plate D 181 exhibits a streaked birefringence pattern between crossed polaroids, as shown in Fig.4(c), which corresponds to streaks of yellow fluorescent Type II diamond in the Type I plate. The close similarity of these streaks to the pattern of streaks in Fig.4(d) of the x-ray topograph of the same specimen is remarkable. Several such examples can be seen by examining the publications from Prof. Raman's laboratory in 1943-45, on a large number of diamond specimens from his collection.

In fact, it was Professor Raman who suggested the name 'x-ray topograph' for such a representation of the variation of x-ray reflection intensity over the area

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of a crystal plate. At that time (1944), I was not aware of any earlier work of a similar nature, although in the 1960's, I came to know of the work of Berg [26,27], who however had used surface ("Bragg type") reflections for this purpose by using the line focus of an x-ray tube. However, he called his pictures 'images' and, to the best of my knowledge, the word 'x-ray topograph', which is widely used nowadays, was employed by me for the first time in 1944. Also, our technique of using white radiation was quite different from Berg's technique using monochromatic radiation.

In fact, I went further, and using different specimens of diamond from Raman's collection which were all blue-luminescent (Type I), but had different intensities of fluorescence, I could show [28] that the width of x-ray reflection for Cu Kα had a positive correlation with the intensity of luminescence. The luminiscence is known now-a-days to be caused by inclusion of impurity atoms like nitrogen, which would definitely lead to imperfections, and the correlation is understandable.

(b) Degree of perfection using polarized x-rays

As is well known, R_y is proportional to $|F|$ for a perfect non-absorbing crystal, and proportional to $|F|^2$ for an ideally mosaic crystal. Hence, if polarized x-rays with different azimuths are used, the ratio $\rho = R_{y\perp}/R_{y\parallel}$ will be different, namely

$$\rho_P = \cos\theta \quad \text{for the perfect (non-absorbing) case} \qquad (23a)$$

and

$$\rho_M = \cos^2\theta \quad \text{for the ideally imperfect case} \qquad (23b)$$

If the crystal is absorbing, $\rho_{PA} < \cos\theta$, but still greater than $\cos^2\theta$ for ρ_{MA}. Hence, if we measure ρ_C for a crystal of unknown degree of perfection (Δ), then we can define Δ by

$$\Delta = \frac{\rho_C - \rho_{MA}}{\rho_{PA} - \rho_{MA}} \qquad (24)$$

This idea can also be applied for any azimuth ϕ of polarization. A polarization spectrometer to check this idea was built by Ramaseshan and me in the early

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1950's [29, 30] using the 440 reflection of calcite (Bragg angle $43^{\circ}58'$). The technique was further developed and applied for assessing the degree of perfection of a crystal in various ways by K.S. Chandrasekaran in my laboratory in Madras (to which I had moved) in the succeeding years. A brief review of these studies is available in [31]. (It is interesting to note that, by using the 311 reflection of copper (Bragg angle $\theta = 45^{\circ}6'$), Chandrasekharan was able to get almost perfect polarization [32], and the paper, reporting the results thus obtained, was highly commended by Prof. Compton in a letter to us in Madras.) This polarization technique was also applied by S. Chandrasekhar in Prof. Bragg's laboratory in London, especially for the evaluation of extinction corrections — see [33] for a review of these.

(c) Mosaic versus perfect crystals

In the above studies of K.S. Chandrasekharan, ρ_{PA} from theory, was always calculated using the relevant formulae obtained using the dynamical theory such as those reported in [17], [18]. In this connection, the question was raised whether ρ_{PA} can be larger than ρ_{MA} under any conditions. The answer, in the case of an internal reflection ("Laue case") was 'yes', as obtained from theory, provided the crystal thickness was of the right order. This apparently strange result was published in Nature by myself and Parthasarathy [34], which contained the curves of log ρ_{PA} and log ρ_{MA} versus thickness (t) for the practical case of the 211 reflections of calcite. The same year, we carried out experiments, using near perfect and mosaic crystals of calcite of various thicknesses, and obtained results confirming the theoretical values almost completely. These were presented at a Symposium on Crystallography and Crystal Perfection held in Madras in 1963, which was attended by Bormann, Hemminger and Kato, and was published in its Proceedings [35]. (See Fig. 5, reproduced from Ref. [35]). The theoretical curves along of this figure were also given in Ref. [34].

By this time, the interests of our laboratory at Madras had turned towards the structure of proteins and other biopolymers, and we stopped working on the dynamical theory and crystal perfections. However, recently in 1978, my attention was directed to a paper by S.V. Wilkins [36], forwarded by Sir Peter Hirsch to the Royal Society, which mentions, as being new, the theoretical result that "if absorption and anomalous reflection are both large, then for some range of parameter values the integrated reflectivity for a perfect crystal can exceed that for an ideally mosaic crystal" (italics as in the quotation). Surprisingly, neither of our above two papers [34, 35], where this had not only been calculated from theory, but even established experimentally (fifteen years earlier), are mentioned in this paper.

I hope that this brief review of our contributions in the field of x-ray studies of crystal perfection will be of interest to workers by bringing to their attention some unnoticed results and observations related to these.

Acknowledgements

I am grateful to the University Grants Commission, India, for a generous grant for "Studies in Epistemology", which enabled me to write this review. I also thank Prof. S. Chandrasekhar of the Raman Institute for assistance in arranging for the reproduction of Figs. 1 to 5, and Mr. Manjunath for secretarial assistance.

References

1. Lord Rayleigh / Proc. Roy. Soc. Lond. A93, 565 [1917].
2. C.G. Darwin / Phil. Mag. 27, 675 [1914].
3. P.P. Ewald / Ann. Physik 49, 1 and 117 [1916].
4. P.P. Ewald / Ann. Physik 54, 510 [1917].
5. A.H. Compton and S.K. Allison / X-rays in Theory and Experiment, van Nostrand, New York, 2nd Edn, 1935 .
6. J.A. Prins / Z. Physik. 63, 477 [1930].
7. L.B.W. Joley / Summation of Series, Chapman & Hall, London [1925].
8. G.N. Ramachandran / Proc. Indian Acad. Sci. A 16, 336 [1942].
9. C.V. Raman and D. Krishnamurthy / Proc. Indian Acad. Sci. A36, 321 [1953].
10. G.N. Ramachandran / Proc. Indian Acad. Sci. A20, 100 [1944].
11. W.H. Zachariasen / Theory of X-ray Diffraction in Crystals, John Wiley, New York, 1945 .
12. G.N. Ramachandran / Acta Cryst. 1, 155 [1948].
13. G.N. Ramachandran and P.B. Hirsch / Acta Cryst. 3, 187 [1950].
14. G. Borrmann / Phys. Z. 42, 157 [1941].
15. G. Borrmann / Z. Physik. 127, 297 [1950].
16. M. von Laue / Acta Cryst. 2, 106 [1949].
17. G.N. Ramachandran and G. Kartha / Proc. Indian Acad. Sci. A35, 145 [1952]
18. G.N. Ramachandran / Proc. Indian Acad. Sci. A39, 65 [1954].
19. H.N. Campbell / J. Appl. Phys. 22, 1139 [1951].
20. G.N. Ramachandran / J. Appl. Phys. 23, 500 [1952].
21. P.B. Hirsch / Acta Cryst. 5, 176 [1952].
22. N. Kato / J. Phys. Soc. Japan 10, 46 [1955].
23. Z.G. Pinsker / Dynamical Scattering of X-rays in Crystals, Springer-Verlag, Berlin, [1978].
24. G.N. Ramachandran / Proc. Indian Acad. Sci. A19, 280 [1944].

..17

25. G.N. Ramachandran / Current Sci. (India) 13, 156 [1944].

26. W.F. Berg / Naturwissenschaften 19, 391 [1931].

27. W.F. Berg / Z. Krist. 89, 286 [1934].

28. G.N. Ramachandran / Proc. Indian Acad. Sci. A20, 245 [1944].

29. S. Ramaseshan and G.N. Ramachandran / Acta Cryst. 6, 364 [1953].

30. S. Ramaseshan and G.N. Ramachandran / Proc. Indian Acad. Sci. A39, 20 [1954].

31. K.S. Chandrasekharan / Acta Cryst. 12, 916 [1959].

32. K.S. Chandrasekharan / Proc. Indian Acad. Sci. A44, 387 [1956].

33. S. Chandrasekhar / Advances in Physics. 9, 363 [1960].

34. G.N. Ramachandran and R. Parthasarathy / Nature 196, 1306 [1962].

35. R. Parthasarathy, G.N. Ramachandran and M. Mallikarjunan / In "Crystallography and Crystal Perfection" Ed. G.N. Ramachandran, Academic Press, London, [1963].

36. S.W. Wilkins / Proc. Roy. Soc. Lond. A364, 569 [1978].

Figure Captions

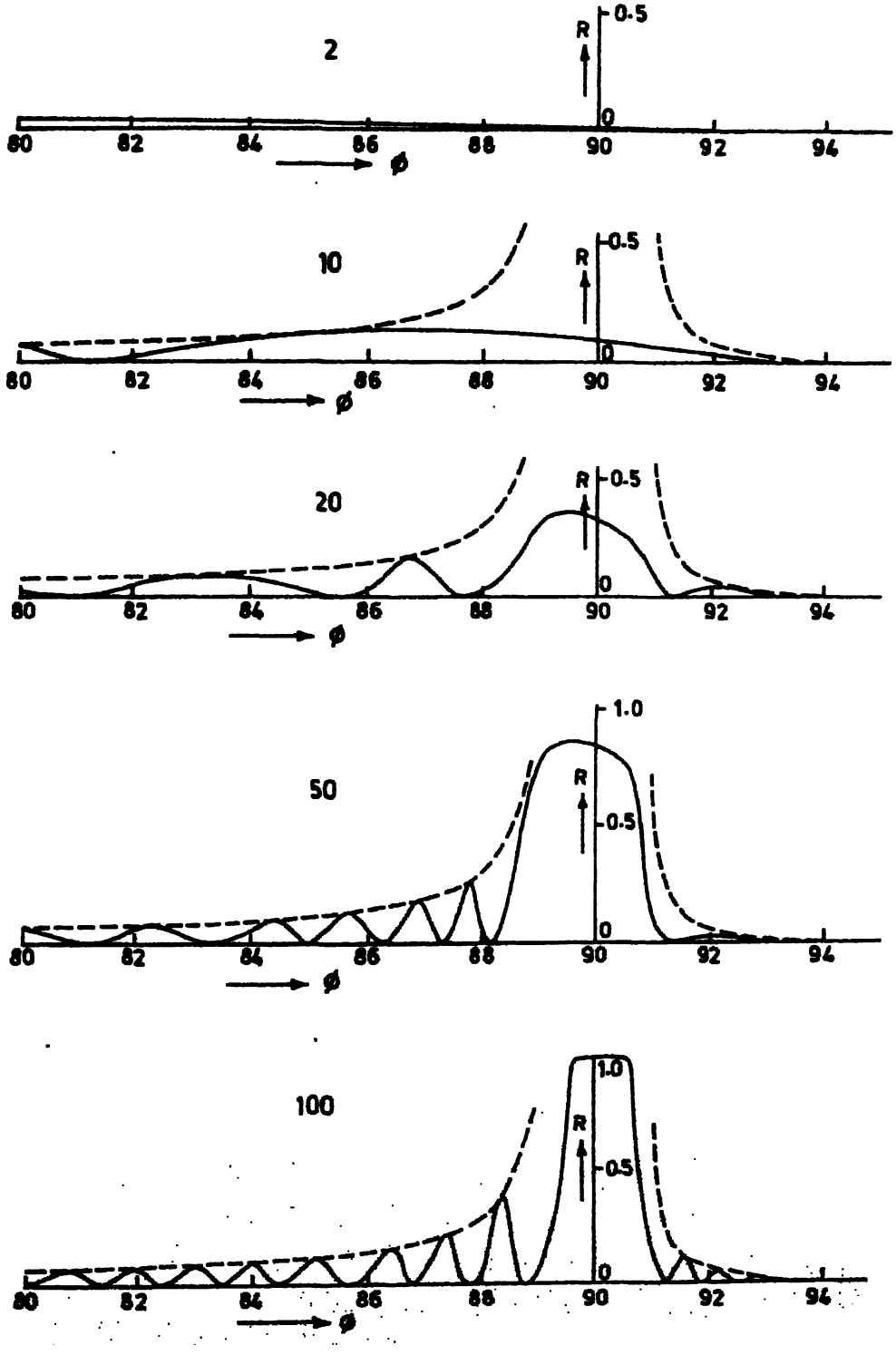
Fig.1. Variation of reflection coefficient ($= |R_1/T_1|^2$) with angle θ for a typical example, having the number of stratifications (n) varying from 2 to 100. Note that, although the central maximum increases in intensity, its width reaches a lower limit, and does not decrease indefinitely with increase of n.

Fig.2. Observed reflection "spectra" from a multiply twinned $KClO_3$ plate, for different polarization states. Note the larger width of the central maximum than that of the subsidiary maxima, and also the asymmetry of the side bands, as expected from theory.

Fig.3. "Reflection" (full line) and "anti-reflection" (broken line) peaks as calculated from theory for the 211 internal reflection of calcite of sufficiently large thickness, corresponding to Campbell's experiments. Note the shift in angular setting between the two peaks.

Fig.4. (a) Luminescence pattern and (b) x-ray topograph, of D 180, a blue-luminescent, Type I diamond plate; (c) Birefringence pattern (under crossed polaroids) and (d) x-ray topograph, of D 181, a Type I diamond plate, with Type II inclusions. The correspondence between (a) and (b), and between (c) and (d), is worth noting (See text).

Fig.5. Variation of the logarithm of ρ_{PA} and ρ_{MA} with t for the calcite 211 internal reflection. Note that the former can be larger than the latter, and that the experimental points are in support of this.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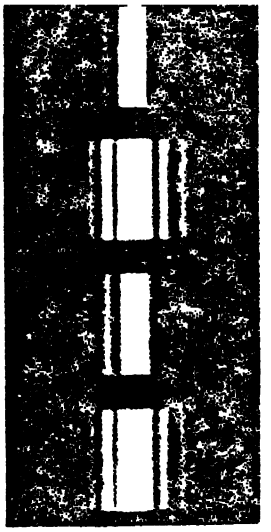
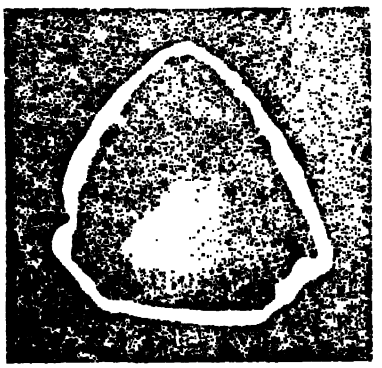


Fig. 2



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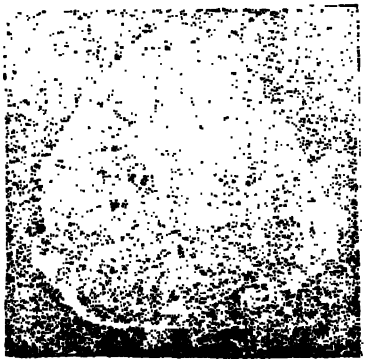

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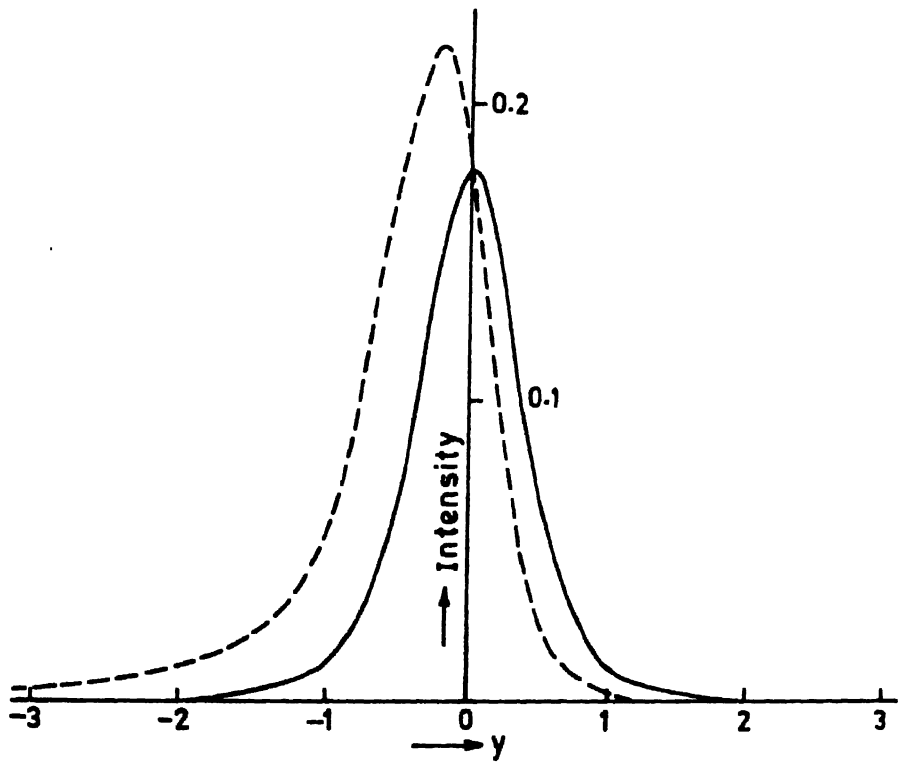
Fig. 4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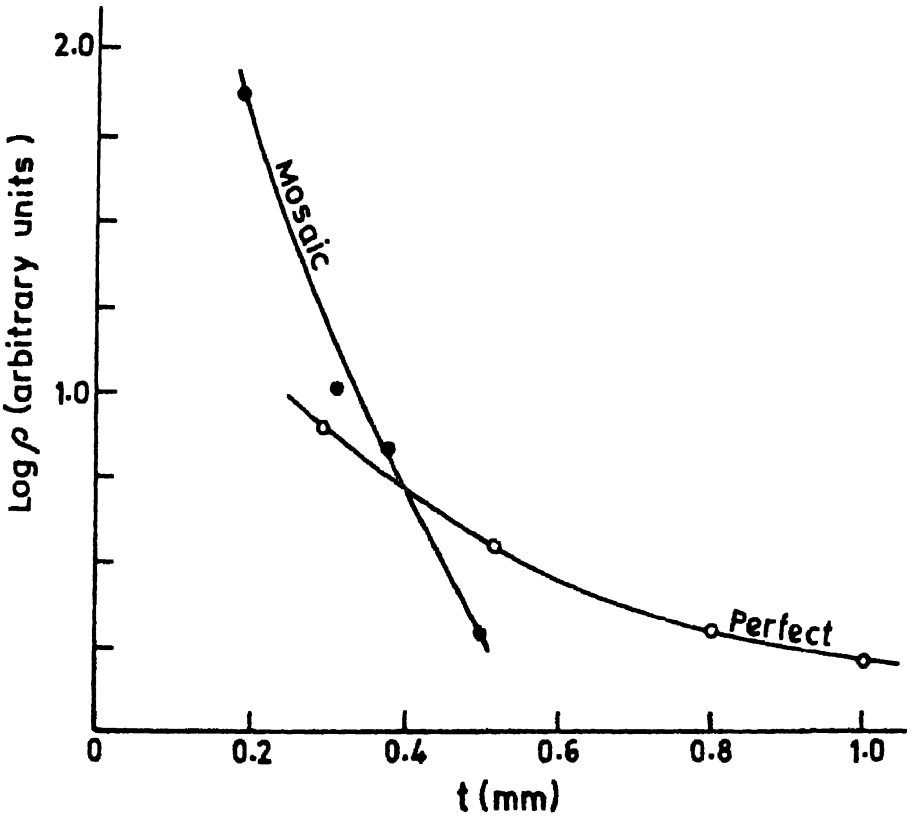
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Mathematical Philosophy Group

(Summarized Report for 1978-82)

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MATHEMATICAL PHILOSOPHY GROUP

(Summarized Report for 1978-82)

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MATPHIL Reports No. 27, December 1982

Studies made in the Mathematical Philosophy Group (1978-82)

Dr. Ramachandran went for a visit to the National Institutes of Health, Washington D.C for a year from 1977-78 as Fogarty International Fellow, and during this period he had intense discussions on molecular biophysics and molecular biology with workers in various laboratories in USA. As a result of this he felt that one could not work on the advancing front of knowledge in these subjects (even from the theoretical point of view) with the limited facilities for computation that is available in India. Also, the Molecular Biophysics Unit which he had built up in Bangalore had reached an excellent viable position, with three or four workers of international standard, so that his leadership was no longer necessary for the Unit. In view of all these, he decided to change his subject of study and decided to work on some problems in the fundamentals of science rather than on any particular branch like molecular biophysics. This change over was approved by the Indian Institute of Science and he was given a small group called Mathematical Philosophy Group with two or three assistants and plenty of funds for books and computation.

During the last four years since 1978, the work of this

Mathematical Philosophy Group has been directed mainly towards Mathematical Logic and partly towards studies on the Theory of Knowledge in which the ancient Indian approach to this subject was also followed up. The work done was mostly published in the form of 25 articles turned MATPHIL Reports 1 to 25 which are listed at the end of this short summary of the activities of this group. A few papers have been sent to journals and these are also listed along with the reports.

The studies can be most conveniently divided into the following parts:

1. Vector-matrix representation of logic and its application to computerization of logic.

2. Essays and translations of ancient Indian texts in the light of modern philosophy, especially epistemology.

3. Pure mathematical studies on Fourier Transforms.

4. Studies on X-ray crystallography directed towards the development of a new technique of Structure Analysis.

Mathematical Logic: It is well-known that the simplest type of logic, called Propositional Calculus (PC) is based on two states of any logical sentence, namely true (T) and false (F). While attempting to represent these states by the presence of voltage in two lines, designated α and β, of an electronic circuit, it came out that there must be two more states that must be included — namely doubtful (D) and impossible (X). The (α β) notation for the four states are thus, T = (1 0), F = (0 1), D = (1 1) and X = (0 0). Then, one can talk of Boolean 2X2 matrices as interconnecting such vectors. This gives a satisfactory mathematical representation of all the logical connectives like "and", "or", "if", "nand", "nor", "equivalent" etc. Any logical statement becomes an equation in Boolean algebra of genus-2 (BA-2) and the process of logical analysis, using the mind for testing the validity of an argument, is very simply done by working out multiplications and additions and checking the result for (α β). It gives either truth, falsehood, or the possibility of there being either truth or falsehood (which cannot be resolved with the data given) which is the picture of state D = (1 1) in this logic. The idea of universal doubt and its clearance to give T or F was the central basis of the epistemology of Jaina philosophers of ancient India. Their so-called "syād-vāda" was based on these ideas. Therefore, the name SNS standing for syad-nyāya-system

has been given to the extended propositional calculus of logic which can be represented isomorphically by BA-2 (syad = may be ; nyaya = logic in Sanskrit).

The impossible state X = (0 0) serves the purpose of checking for contradictions. If the output of an equation in logic is (0 0), then either one or more statements that led to it are wrong, or the argument itself is invalid. The precise place where the contradiction originated can be tested by reversing the argument. The existence of X is detected by making use of a new logical operator $\underset{\sim}{V}$ (vidya) (different from $\underset{\sim}{A}$ (and)). This operator $\underset{\sim}{V}$ also seeks out the common state that is present from two statements giving the logical state of the same term — $T \underset{\sim}{V} T = T$, $T \underset{\sim}{V} D = T$, $F \underset{\sim}{V} D = F$, $D \underset{\sim}{V} D = D$ etc. This again is a classical concept in Ancient Indian philosophy— Knowledge (or Vidya) is obtained by the resolution of doubt.

These ideas of SNS have been written in a computer program and have also been incorporated in an electronic machine on which logical arguments can be tested.

The above ideas developed for PC has been extended to Quantified Predicate Logic (QPL) by working out an isomorphism between it and Boolean Algebra of Genus 3 (BA-3). The six-element Boolean vector (λ) (γ' δ' ϵ') (α β) of standard QPL is converted

into a canonical form (γ δ ϵ) of BA-3 and then it is discovered that QPL has four more states than the four standard ones — namely "all" ($\forall$ = (1 0 0)), "none" ($\underline{\phi}$ = (0 0 1)), "not all" (Λ = (0 1 1)) and "there exists" ($\exists$ = (1 1 0)). The algebra of their interconnections is via 3X3 Boolean matrices, of which there are 64 of each kind — e.g. $\mathbb{A}(1, 6)$ corresponding to " $\forall$ and $\exists$ ". In addition the vidya operator $\underset{\approx}{\vee}$, is defined in this also as $a \underset{\approx}{\vee} b = (a_\gamma\ a_\delta\ a_\epsilon) \otimes (b_\gamma\ b_\delta\ b_\epsilon)$. This leads to a new state "some" ($\leq$ = (0 1 0)) in QPL. We call the logic containing this and other new states isomorphic to all eight vectors of BA-3, as extended QPL (EQPL), and the principal ideas of EQPL have been worked out.

Here again the state "some" ($\equiv$ doubtful, but neither true, nor false) had been postulated by the Jaina philosophers of two thousand years ago, and given the name "avaktavya" (indescribable) in addition to the two common states "true" and "false".

The above have been written as Fortran programs. Studies are proceeding to make the computer itself reverse an argument and discover consistency or contradiction of any set of arguments in SNS and/or QPL, and also to point out the exact place of origin of inconsistency.

Epistemology: The above studies on logic led to the consideration of problems in epistemology. This approach is in the spirit adopted by ancient Indian philosophers, who never separated logic from the information content in a statement — just as grammer cannot be completely divorced from knowledge. A study of logic alone is barren; but logic can give intimate understanding of some of the puzzling aspects of knowledge. Thus, considering the nature of Supreme Knowledge, i.e about the Supreme Being that controls the Universe — we get into paradoxes. We know it, yet we do not know it (Kena Upanishad). To the question "Do we know it?" the answer is "no" and "yes" at the same time. If we stick to pure logic, any statement must be either true or false and the above statement becomes a contradiction, since both its affirmation and negation are said to be valid. However, SNS logic has a state in which the knowledge may be either true or false, without being contradictory. The negation of this state D is itself again D so that we get the equation $D = \neg D$. Thus, the introduction of the doubtful state into logic immediately resolves the apparent paradox of statements in kena upanishad, which have always puzzled the scholars of the Theory of Knowledge. Here is a case where the Indian philosophers knew the essence regarding such a logical state, without studying explicitly about it.

In the same way, Jaina philosophers had understood the QPL state "some", to which they gave the name "avaktavyaya". In the present century, the existence of theorems, which can neither be proved to be false nor proved to be true, was demonstrated by Gödel; and this is considered to be one of the highlights of modern logic. The consequence for epistemology is whether this is a paradox in the theory of knowledge — that knowledge can never be complete and theorems exist that can be neither proved nor disproved. By introducing the state "some" (which is essential for isomorphism with BA-3), the Gödel state (as we may call it), has been made into an acceptable state of EQPL. Neither the logic, nor the knowledge dealing with such theorems or statements, makes Knowledge itself defective in any manner. In fact, if one goes to BA-7 and higher order Boolean algebras, then very many more surprisingly complicated states can be included in logic.

Thus, in summary, there is much to learn from ancient Indian philosophy even today to improve the subject of epistemology.

In this connection, the Kena Upanishad has been translated into English verse and an article has been written on it, and on deduction according to Indian logic.

Fourier transforms: Dr. Ramachandran was trained in the subject of Fourier transforms when he worked under Prof. Sir C.V. Raman in the 1940s. As is well-known, diffraction theory is nothing but Fourier analysis, and various problems in diffraction which he worked with Raman enabled him to study Fourier transform theory rather intimately from the applied mathematics point of view. During the last couple of years, he and his group extended the idea of differentiability of order n to the situation where $n \longrightarrow \infty$. It was shown that, if the differential coefficient $d^n y/dx^n$ exists for $n = \infty$, then the function must be the Fourier transform of a "physical function". By a physical function is meant a function that is absolutely integrable and which is bounded in its support. Both these conditions are true of any real physical body, because it must be finite in dimensions, and finite in the value of its mass (mass being used as a word to indicate any physically measurable quantity). A number of studies were made on the Fourier transforms of physical functions, and it was shown, for instance, that such a function must also be infinitely oscillatory.

X-ray crystallographic structure analysis: Following up the studies on Fourier transforms, a new approach towards the initial steps in crystal structure analysis was developed.

This directly uses the intensities of reflections and approximates the structure by a grid of atoms at positions having coordinates equal to rational fractions of the unit cell dimensions a, b and c. Only the strength (m_i) of the atoms i at (x_i, y_i, z_i) are allowed to change and a standard least squares type of calculation was found to reduce the R-value regularly even down to 0.25 or less, for two-dimensional structures, starting ab initio with random m_i's. The essence of the method seems to be that both the original structure and the grid-approximated structure must have a large temperature factor B in the initial stages. The method is still under development; but it appears to show promise.

A PHYSICIST'S VIEW OF MATHEMATICS

(Summary of the Lecture delivered at the Punjab University, Chandigarh, in November 1981)

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MR No. 28, December 1982

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MATPHIL Reports No. 28, December 1982

A Physicist's View of Mathematics*

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As we all know, the interaction between physics and mathematics has been to the mutual benefit of both right from the early dawn of civilization. I will not deal at all with the early development of science in various countries like Greece, India, China etc., but deal mainly with the situation as it exists today, when every physicist has to be a mathematician to do good physics, whether it is purely theoretical physics, or experimental physics based on observational data. In view of this, I shall deal with three main types of mathematics that a physicist always needs, namely,

(a) Mathematical Physics.

(b) Physical Mathematics which is a subdomain of pure mathematics, not all of which is needed in physical theory.

(c) Physical Basis of Mathematics. Under this I shall try to show that the purest of pure mathematics has its basis developed essentially from physical observational techniques.

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*This article is a summarized version of the talk with the above title delivered at the Punjab University, Chandigarh, about a year ago, under the auspices of the Indian Physics Association. The article will highlight the main points discussed and will not contain all the details of the original talk.

(a) Mathematical Physics: Physicists always require a precise formulation of their theoretical ideas for working out the consequences of such ideas. Although there have been great scientists in the last century who did much of their physical deduction purely from ideas and concepts (for example, Michael Faraday for electromagnetism), it is always convenient to convert any physical theory into a set of formulae expressed in mathematical symbols and thereafter treat these as problems in mathematics for obtaining the solutions that are required — namely the consequences whose nature and magnitude have to be obtained. In this sense, mathematics is used as the tool by the physicists. If I may say so, if, as is often said, mathematics is the Queen of Science, physics should be called the King of Science who rules over the queen. In fact, many branches of pure mathematics such as trigonometry, algebra, differential and integral calculus, all had their origin in the requirements for discussing in a precise manner various observations in science. Perhaps, the culmination of these was the Lagrangian formulation of mechanics which, along with Newton's Law of Gravitation explained almost everything that was known at that time in the field of celestial mechanics.

In this connection, a perusal of Fig. 1 will be very interesting to indicate how observational data are converted

into a theoretical formalism and then used for deducing consequences. If all the consequences agree with observation, then everything is good; but some of them will not be included in the formalism first worked out, in which case these are added to the original set of observations to reformulate the theory so as to contain them also and once again fresh mathematical theories worked out. This process as indicated by a do-loop in Fig. 1, is continuously to be repeated, and very simple considerations will show that it can never be completed. It is like what Newton said — namely that he was only a child gathering pebbles on the seashore while the whole of science was there out in the ocean.

To indicate an example of the going over from physics to mathematics and back to physics again, we shall mention only one or two cases. As is well known, physics was considered to have been brought to a completely satisfactory state by the end of the 19th Century. However, the observation that the perihelion of mercury was precessing and cannot be explained by Newtonian mechanics was a dilemma for scientists for some time. The solution to this did not come from pure mathematics because as I had said earlier, mathematics needs the background of observational data to complete its full development. (I am sure most mathematicians will disagree with this, and say that mathematics is a process of

mind and does not depend upon observation for its development). In this particular case, the Special Theory of Relativity and, ever more, the General Theory of Relativity of Einstein, which were essentially physical ideas, founded on mathematics gave a satisfactory explanation of most of astronomy and dynamics that was known at that time. It is a moot point whether Einstein's theory is in physics or in mathematics. The two are intimately intertwined and while the ideas of the theory came from the physicist's mind, the formulation of them for use by others was possible only after they were fully converted into mathematical equations. As everybody knows, the idea that space and time are interchangeable between different Lorentz frames was an enigma for many scientists of the 1900's. Even more, the curvature of space in the general theory was something that only the experts knew and could manipulate with. However, the beauty of the theory is best appreciated by looking at the simplicity and the generality of the mathematical framework. In this sense, mathematics gives a covering and a beautiful dress to physics in order that it can go about and be of service to scientists in general.

(b) Physical Mathematics: Under this heading "Physical Mathematics" we shall merge two topics which are closely interrelated, one of which is pure mathematics and the other is essentially pure physics

in the realm of mathematical physics. Talking of Fourier transforms, it can be considered to be a purely mathematical subject. In that sense, we take two spaces — the real space x and the reciprocal space X — such that we get the well-known Fourier transform equations

$$F(X) = \int_{-\infty}^{+\infty} f(x) \exp(i2\pi Xx)\, dx \qquad (1)$$

$$f(x) = \int_{-\infty}^{+\infty} F(X) \exp(-i\, 2\pi xX)\, dx \qquad (2)$$

As is well-known, the idea of Fourier transforms first appeared as Fourier series for a periodic function for which the first of the above equations takes the form

$$F(H) = \int f(x) \exp(i\, 2\pi H\, x)\, dx \qquad (3)$$

and the second becomes

$$f(x) = \sum_{H=-\infty}^{+\infty} F(H) \exp(-i\, 2\pi H\, x)$$

and the function $f(x)$ is repetitive with a period of unity. The subject arose from a study of periodic phenomena and was

used in the conduction of heat, vibrations of strings and of bodies in general which have periodic variations.

The mathematical theory of Fourier transforms was very well established even a century ago; but yet it had to incorporate new types of functions during the last fifty years. This was essentially in the field of quantum mechanics, wherein Dirac introduced his famous δ-function, $\delta(x - a)$, and the Fourier transform of it has the form $\exp i 2\pi Xa$. The δ-function, from its very definition, is a well understood "physical function" of a quantity which exists only at the point a and whose total "mass", or integral, from $(a - \delta)$ to $(a + \delta)$ is unity. However, it is not bounded in value and does not come within the range of orthodox mathematics.

We have used the word "physical function" in connection with δ-function. A very general definition of a physical function is one for which $\int_{-\infty}^{+\infty} |f(x)|\, dx$ is finite, and also for which $|f(x)| = 0$ for all $|x| > a$, where a is finite. In simple words, this means that the object has finite extension in space and its density integral, or "mass", is finite. As we know, all objects thought of in physics are of this type, although both forward Fourier transforms and inverse Fourier transforms use integrations from $-\infty$ to $+\infty$.

Some of the theorems connected with Fourier transforms of physical functions are implicit in theoretical physics. The process of obtaining the Fourier transform is sometimes called "harmonic analysis" as it gives the values of the amplitude of the waves whose superposition gives the object. However, it was only in the 1920s that the full application of harmonic analysis was made to all matter and its interaction with radiation. It first arose as an experimental, or physical, idea due to de Broglie, who said that a particle with a momentum p has a wave nature associated with it with its wave length $\lambda = h/p$. It then stands to reason that the distribution of the mass of the particle can be obtained as a superposition of all the possible waves that occur associated with it. When the idea is applied in mathematical terms, it is found that it is not the functions $\rho(x)$ and $\rho(p)$, which express the densities in the coordinate space and in the momentum space, which are Fourier transforms of each other. Instead, they are related in terms of two functions $\psi(x)$ and $\chi(p)$ (both of which are complex) and which are related according to equations (1) and (2), and $\rho(x) = |\psi(x)|^2$ and $\rho(p) = |\chi(p)|^2$. This leads almost immediately to the famous uncertainty principle of quantum mechanics, namely

$$\Delta x \ \Delta p \leqslant \frac{h}{2\pi} \qquad (5)$$

It is not very difficult to derive most of the basic and essential equations of quantum mechanics from just the above

mathematical interpretation of de Broglie's essentially physical concept of the wave nature of matter.

The above arguments will indicate that while mathematical equations can be written, the physical interpretation of these is what gives them life and substance, and very often these physical ideas may lead back to improvements or new results in mathematics itself. We shall mention only one such example, which has been obtained by our laboratory during the last three years. This is that, if the function f(x) (which can be extended to three dimensions) is absolutely integrable and is of bounded support, then, the Fourier transform function F(X) is infinitely differentiable, and vice versa. We shall not define infinite differentiability except saying that

$$\lim_{n \to \infty} \frac{d^n F(X)}{dX^n} = \text{finite} \qquad (6)$$

This concept which is a very eminently physical concept — differentiation is very well understood as a physical operation — has several ramifications connecting it with the theory of complex variables and what are known as entire functions of the exponential type in functional analysis. In fact, we have also shown that Fourier transforms of physical functions are infinitely oscillatory and some derivative of the function F(X)

has finite amplitude of oscillation even as $X \rightarrow \infty$. In fact this theorem is directly connected with the property of the function $f(x)$ (of which it is the Fourier Transform), namely that the derivative of some order n ($f^{(n)}(x)$) has a δ-function distribution as part of it.

As is well-known, both the δ-function and its Fourier transform are not acceptable as "functions" according to the rigorous pure mathematics; but it is implicitly accepted by every physicist that a physical function has a Fourier transform. We feel that our theory actually proves this with mathematics of fairly high rigour. (The so-called theory of "Distributions" of Schwartz, and of "Generalized Functions" of Gel-Fand are available, but they are based on complicated mathematics, while our theory is based on simple physical principles, expressed in a suitable mathematical formalism.)

(c) Physical Basis of Mathematics: This brings us to the question, "Is the full machinery of rigour of pure mathematics necessary for physical applications?" Associated with this, we shall ask the question, "Which is earlier in its fundamentals—Physics or Mathematics?" It is our view that it was physics that led to mathematics and that concepts in mathematics are

abstractions, made by thought, of physical phenomena. Take for example, the simplest concept of "number"— 1, 2, 3, 4 etc. Actually one can only count one book, two books, three books etc.; or one stone, two stones, three stones etc. But the concept of 1, 2, 3 etc., as numbers which have certain properties common to all these examples is an abstraction of the mind from observation of matter. We wish to assert that the mathematical concept could not have arisen but for the observation of nature by the senses. The sense impressions that went into the brain were then subjected to analysis and concepts were created, understood, transmitted and made into a different discipline— namely mathematics.

Actually, every branch of mathematics has arisen essentially from physical observations. Thus, Euclid's geometry came out of the examination of objects and their shapes and extensions. Algebra arose from numbers by one more degree of abstraction and the association of symbols like x, y, z to any number whatsoever having certain restrictions. Later developments in mathematics were products of mental imagination but always one can ask the question, "Does not each branch of mathematics have a physical basis as origin?" For example, abstract group theory, which is a branch of algebra, has its correspondence in the

theories of symmetry of real or imaginary objects, and the elements of a group can be represented by rotations in n-dimensional space. Here the distinction between pure mathematics and applied mathematics, or physics, is very thin, because many fine theorems on group theory have been suggested by the representation of it in terms of rotation and reflection operators, which are again represented by matrices acting on vectors. In fact, for many physicists, pure group theory is something which justifies all that they do, although the things with which they operate are physical in nature and even understood a imagined as such.

This brings us to the question whether all of mathematics has in fact originated from physics. Some very recent work in our group has indicated that even the purest of pure mathematics— namely mathematical logic — can be given a completely understandable and picturizable appearance by representing logical states and logical connectives by algebraic elements and operators acting on them, which again can be interpreted by Boolean vectors and Boolean matrices multiplying such vectors. We have shown in fact that the whole of logic can be described in terms of Boolean vectors and matrices. While doing this, the method of approach that is adopted is that of a physicist — namely thinking of logic as the "Science" of Reasoning or Thought, and bringing

out physically each law that holds in this science, and then giving the concept a "local habitation and name" in terms of Boolean vectors and matrices. In other words, logic can be shown to be consistent and to have a coherent existence; but what the laws are and how they are interrelated are matters not of pure thought alone, but are obtained by the method of analysis of a physicist — namely of observation, codification, interpretation and symbolization. The connections between the symbols in mathematical form and the logical terms and connectives can be obtained in a unique way, by using the so-called "Theory of Relations" (which again can be formulated as a physical theory).

It is in the light of these that we wish to state that mathematics does not antidate physics, but that mathematics arose out of a rationalisation and symbolization of every type of observation including the observation of itself, namely of the Laws of Reason.

CRYSTALLOGRAPHY IN MOLECULAR BIOPHYSICS

(Summarized account of the Sir C.V. Raman Medal Lecture delivered at Tirupati on Jan. 1, 1983)

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MATPHIL Reports No. 29, December 1982

Crystallography in Molecular Biophysics*

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1. Chemical Structure and Physical Structure of Biomolecules

I am deeply grateful to the President and Council of INSA for the honour they have done me by awarding me the Sir C.V. Raman Medal, which I believe has been given in appreciation of the contributions made by our laboratory in the fields of molecular biophysics and crystallography. The pleasure is doubly so, since I was myself a disciple of the revered Professor Raman and learnt the essentials of crystallography under his guidance. The field of molecular biophysics has now become a large one; but its growth has been due to a large extent to the rapid advances in X-ray diffraction techniques that have taken place during the last 20-30 years. In this lecture, I shall try to give you a brief account of how chemical physics and physical chemistry can contribute much to our understanding of life processes in organisms, — not only in their normal state, but even to find the cause and cure of many diseases. It has been a good fortune of our laboratory to have entered this field of molecular biophysics practically

*Summarized account of the Sir C.V. Raman Medal Lecture to be delivered at Tirupati on January 1, 1983.

at the beginning of the exponential growth of this subject starting from the early 1950's.

As everybody knows, the chemical behaviour of a material becomes fully understandable only when its molecular structure, and electronic charge distribution over its volume becomes known. What else is better for probing this than the techniques employing various types of physical properties — ultra-violet spectroscopy, infra-red and Raman spectroscopy, nuclear magnetic resonance, optical rotatory dispersion, and last, but not least, X-ray diffraction techniques. It is obviously impossible even to point out the role that each of these techniques play in biomolecular structural research. Therefore, this talk will be restricted, even within the field of molecular biophysics, to the analysis of the shapes or conformations of biomolecules and that too, essentially as determined via theoretical and crystallographic techniques.

In doing this, first, we shall indicate how information about the detailed molecular architecture of biomolecules (both small molecules, oligomers and polymers), obtained from crystallographic and other techniques, are translated into information of value to biology. The word molecular biophysics for this is clearly appropriate because it is the knowledge about biomolecules studied by physical techniques that has

contributed to much of our knowledge about the chemical reactions that takes place in biological systems at the molecular level. In the light of this, we shall use two terms —"physical structure" and "chemical structure" —for distinguishing between two different aspects of biomolecular structure that are needed for this purpose. Of these, what is available at the beginning is the chemical one —i.e. the nature of the atoms that are contained in the molecule and of the chemical linkages between these. These data have been connected with the expected biological chemistry of the molecules by organic chemists and biochemists. The physical features of the molecule, on the other hand, deal with the detailed three-dimensional description of the molecule, in terms of bond lengths, bond angles and dihedral angles. The most suitable technique that gives these is X-ray crystallography which gives these parameters to a remarkable degree of accuracy. However, the data are for the crystallized form of the molecule, while in general, the molecules are in solution in the biological system, or freely interacting with the solvent; and it is the structure under these conditions that is what is wanted.
It is here that the theorist in this field has a very important part to play. By examining and analysing the physical structures observed in various crystals, they derive suitable laws and

they also utilize pure theories in chemical physics to work out the various possible changes in conformation that can lead to the actual biologically active state of the molecule. We shall discuss a few examples of biological fibres (which are, for all purposes, in the crystalline state) and discuss their importance in biochemistry, and we shall also consider interactions between biopolymers and small molecules which are important in understanding not only the basic metabolism of living organisms, but even what happens in pathological conditions and how drugs interact with biological systems.

In the sections that follow much of this will be discussed in a condensed manner, as this written material will only briefly describe the different aspects that will be presented at the lecture. Therefore, complete coverage is not made of the literature of the subject and the figures also have been reduced to a minimum in the text here, although they will be fully illustrated in the actual lecture.

2. Crystallography, the sourcehead of biomolecular theory.

As mentioned above, much of the information regarding the shapes of organic compounds has come from X-ray crystallography. Although organic chemists had reasonably clear pictures of the shapes of many of the smaller biomolecules, the way in which

these fragments are combined together in biopolymers was made clear only by studies starting from about the 1940's. In all these cases, many smaller molecules containing segments of biopolymers, such as dipeptides, tripeptides and so on, were available and crystal structures of these gave the precise dimensions of the bond lengths, bond angles and dihedral angles which characterize these molecular structures. Perhaps, the most important "extract" that had come out of this body of information was the enunciation of the planar peptide unit by Linus Pauling and collaborators. They showed that the peptide unit C^{α}—CO—NH—C^{α} had all the atoms in it in a planar configuration and that the peptide unit can have either a <u>cis</u> or a <u>trans</u> conformation, according as C=O and N—H are pointing in the same direction or in opposite directions. At that time. there was no clear evidence of one of these being more predominant than the other, although very soon the planar <u>trans</u> peptide unit came to be established as the building block of all open chain polypeptides and proteins.

In obtaining these dimensions of the planar peptide unit Pauling used all the available X-ray data of that type. In fact, it is a matter of some theoretical interest (as Prof. Pauling says in his Presidential Address to the Madras Conference on

Biopolymer Conformation in 1967) that he purposely invited Prof. Corey to Caltech for a year, for checking some of his theoretical ideas by crystallography and that "Corey's year in Pasadena turned out to be 30 years so far".

We, in Madras, entered this field of conformational theory in the early 1950's a couple of years after the postulation of the Pauling α-helix and, true to the tradition, we also had an X-ray crystallographic group working on similar biomolecules side by side. There was always been interaction between theoretical biopolymer chemists and the experimental X-ray crystallographers in the development of this subject all over the world. The situation is still exactly the same — theorists sometimes condense the available X-ray information to give new rules for biopolymer structures and other theorists work out possible structures for biopolymers which have not yet been detected and they soon come to be detected by crystal structure analysis — very often not in the polymers themselves, but in some of the smaller molecules forming parts of the polymers. Crystallography is an ever-living subject and there can be no time in biological research when it will be a postdated. I hope I can illustrate some of these as we go along. Here, I may mention a few examples where our laboratory played some part in the progress of the subject.

Thus, the triple helical collagen structure was proposed in the mid 1950's by employing trans peptide units. While the triple helical configuration was in broad agreement with the fibre diffraction pattern, the data were limited in extent; and no conclusive proof could be given. However, since Pro and Hyp are very frequent in the collagen primary structure, and Gly forms one-third of the amino acid residues, it became clear that the related polymers $(Gly—Pro—Pro)_n$ and $(Gly—Pro—Hyp)_n$ must have similar structures to collagen. These were synthesised only a few years later; but it was a welcome surprise when the simpler polymers $(Gly)_n$, $(Pro)_n$ and $(Hyp)_n$ all had a molecular chain conformation very similar to the backbone chain occurring in collagen, as determined by X-ray diffraction. Here is an example where experiment confirms theory and gave a lot of confidence to workers in the field making use of theoretical structure for various problems in biochemistry (although the complete details have not been revealed even today).

The converse, namely of theory predicting some aspects, happened in the case of the structure of polyglycine II, which has three residues per turn in the helix as against two residues per turn in the well-known β-structure of polyglycine I. In this, we predicted that the structure is stabilized by CH. . .O hydrogen bonds in addition to the standard NH. . .O

hydrogen bonds, which were very strong in this polymer. It is very refreshing that during the last five years, good evidence has come, out of infra-red and Raman studies of polyglycine II made by Krimm and collaborators in the University of Michigan, that the CH. . .O hydrogen bond definitely exists in this structure. The consequence of this is that the existence of this type of hydrogen bond should also be taken into account in the calculation of the stabilizing energy of possible theoretical structures.

3. Principles governing the physical structure of proteins and other biopolymers

By the second half of 1950's, most of the standard helical structures occurring in proteins and polypeptides had been brought into light by X-ray diffraction techniques. In most parts, these had been substantiated and verified by other physico-chemical techniques like ORD, IR and Raman spectroscopy. But the question had to be answered as to why they take these structures and not other structures. When does the α-helix occur? When will a protein have plenty of β-sheet structure? When will it have the triple helical structure of collagen, and, when will it be of random structure for a number of peptide units, without the chain taking up anyone of these ordered

structures? These questions were posed in great clarity by the end of the 1950's with many of the structures having been discovered and a good number of small oligopeptide structures (which form parts of these longer protein structures) having also been solved by crystallographic methods. One of the criteria for the occurrence of a suitable secondary structure like an helix is that as many hydrogen bonds should be formed as are possible — for example, all the backbone NH groups are hydrogen bonded to CO groups in the α-helix, while in the collagen helix two in three are suitably bound and the third one is bound <u>via</u> water molecules. While such criteria as the hydrogen bond length (A. . .B) of the hydrogen bond AH. . .B lie within the prescribed elements, and the hydrogen bond angle O = AH A. . .B should be less than 25 or 30° were very useful for constructing the first approximation to the secondary structure involved, precise formulae or techniques for finding the best structure were not available at that time.

This lacuna was filled during the 1960's and one of the earliest, from the point of view of general technique or principle, was developed in our laboratory, leading to the so-called (ϕ , ψ)-plot for a pair of peptide units. In this the peptide unit C^{α}—(CO)—(NH)—C^{α} is taken to be planar and there are only two dihedral angles, namely ϕ about the bond N—C^{α} and ψ

about the bond C^{α}—C, which are capable of variations when one peptide unit is linked to the next. When the allowed ranges of these two dihedral angles ϕ and ψ were worked out, a set of data giving the closed non-bonded contacts that can occur between different atoms in the chain had to be postulated. For this purpose, we examined the available literature on peptide structures and evolved a standard set of contact distances for the various atoms C, N, O, H that occur in these peptide units. This type of plot is well-known now-a-days, and is widely employed not only for polypeptides and protein structures, but also for working out other biopolymers and simpler molecules.

The (ϕ , ψ)-plot contains allowed ranges of the pair of angles (ϕ , ψ) and about three-fourths of the (ϕ , ψ)-plane is thus disallowed for alanine and other amino acid side chains having a C^{β} atom, while it is almost three-fourths allowed for glycine. This is because both the atoms attached to C^{α} are hydrogens in glycine while one of them is at least a CH_2 group in all the other amino acids. It is not necessary to give a detailed description of the consequences for protein structures, because it is available in several reviews. In particular, a review by me and V. Sasisekharan which appeared in Advances in Protein Chemistry, Vol. 23, 1968 contains very detailed information regarding this and the related energy minimization which is discussed below.

Effectively what the (ϕ , ψ)-plot does is to remove all values of (ϕ , ψ) which lead to even one contact A. . .B being less than the extreme limit which was prescribed from the analysis. We also put another limit called normal limit beyond which there is no restriction at all on the permissibility of the conformation. In essence, we effectively took two energy values, —one where the energy begins to rise sharply and another where it becomes impossibly large. Obviously an exact value of the energy would be a better criterion for studying the allowed and forbidden nature of conformations and this idea struck several workers within a couple of years of the appearance of our article containing the (ϕ , ψ)-contact map in J. Mol. Biol, 1963. We shall not discuss this in great detail except to mention that the energy terms contain a van-der-Waals attraction and a sharp repulsion, in addition to electrostatic energy , and torsional potentials. Hydrogen bond energy is not normally used except while working out in full the total energy of a structure which contains several pairs of (ϕ , ψ) and other similar dihedral angles.

The functions connected with energy criteria were all obtained from a large amount of physical-chemical data about peptides that were available and the (ϕ , ψ)-plot obtained in this way appeared almost simultaneously from several laboratories,

including ours, in 1965-66. Two or three interesting consequences for peptide structures might be mentioned here:

(a) Firstly the energy plot had contours very similar to the contact plot at about the region where the energy was rising rapidly, as mentioned above. The contours for a value of energy equal to +5 to 8 Kcal/mol agreed reasonably well with the extreme limits. In this way, the contact criteria were confirmed by energy calculations and since contact calculations are far simpler on a computer, the contact map is used quite widely even now-a-days. In fact, for some complicated structures like polynucleotides and so on, the energy calculations are an exception, and many valuable consequences can be obtained without energy calculations.

(b) The detailed energy calculation of the triple helical structure of collagen indicated that it had a stabilizing energy as good as, if not better than, the α-helix and it is therefore a stable structure. The details of the structure could be worked out with confidence because the mathematical techniques of building molecular chains and claculating their energies were well developed by that time. Some of the more important results so obtained in our laboratory were discussed in the next section.

(c) From two peptide units one could go to three linked peptide units and this immediately gave a rich dividend, in showing that these could take the form of a "bend", whereby the polypeptide chain is reversed in direction and was hydrogen bonded with itself if both the forward and reverse regions are in the straight chain β-configuration, or the collagen-like γ-configuration. This beta turn was first done in the late 1960's by our laboratory, and it has been widely extended and found tremendous use in the building up of protein chains in globular proteins.

(d) This idea of the "beta-bend" was also extended to chains having alternating L and D amino acids and could explain the conformation of some oligopeptide antibiotics involving these amino acids — for example gramicidin A. Most of the different types of helices that were predicted from pure theory have been observed in synthetic polypeptides of this type, such as poly-γ-benzyl-(L, D)-glutamate.

(e) Another basic aspect of the conformation of polypeptides, namely the possibility of non-planar peptide units being present and their energies were also worked out from our group. The genesis of this idea came from a seminar which I gave in Chicago

when Prof. Mulliken pointed out that the rigidly planar peptide unit, as put forward by Pauling and widely used everywhere for building protein structures need not be so, and that variations from planarity could occur. We therefore calculated the energy changes due to variation for the dihedral angle $\Delta\omega$ about the C...N bond, from the exact value of 180° for a planar peptide unit. It was then found that, in addition, the three bonds meeting at the nitrogen atom would also become pyramidal which could be represented by a dihedral angle denoted by $\Delta\underset{\sim}{\hat{\xi}}_N$ (= 0° for the planar unit). Theoretically, using quantum chemistry, we obtained a plot of the variation of energy with $(\Delta\omega, \Delta\underset{\sim}{\hat{\xi}}_N)$ and found that variations in the former could occur upto about 1 to 15° and the latter upto 20° to 25°.

Theory thus confirms the results found in many protein structures where the fit with electron density indicated the need for non-planar distortions.

This small, but significant, variation in $\Delta\omega$ has led to the theoretical prediction, by Chandrasekaran and Jardetsky that a new type of left-handed helix (the δ-helix) can occur for polypeptide structures. This helix is similar to the left-handed α-helix in being a single chain helix, but the

NH groups are pointing upwards in it, unlike being downwards in the α_L-helix. Recently, by work done in Bangalore, the δ-helix has been shown to be more stable than the left-handed ω-helix that had been previously taken to be the correct structure of poly-β-benzyl-L-aspartate. This is a very interesting prediction, which awaits experimental verification by x-ray diffraction and spectroscopic analysis.

4. Nucleic acid conformations

Unlike polypeptides, which have only three types of dihedral angles (ϕ, ψ, ω) for the backbone, nucleic acid chains are more complicated in that they have six dihedral angles. This was pointed out from our laboratory in Madras as early as 1967. During the last few years, the nomenclature for these have been standardized and they are given the symbols α to ζ. The most interesting fact that was dominating the field, until a few years ago, was that all polynucleotides have essentially the Watson-Crick type of right-handed helices for their chain structure. This, however, had the objection that there will be a lot of tangling occurring during reproduction of the DNA chain, since <u>everywhere</u> it had a right-handed twist. During various discussions that took place in Microbiology, Biochemistry and Biophysics Departments at the Indian Institute

f Science, Bangalore, during 1973-75, possible non right-handed elices which could be stable for a nucleotide chain were onsidered. It became pretty clear that if the nucleic acid hain is partly right-handed and partly left-handed, then separation of the two strands did not require untwisting as much as it would be needed if it were wholly right-handed. The problem was studied theoretically by Sasisekharan and coworkers and they discovered that a good stable left-handed structure is possible for nucleic acid chains, and at about the same time, some work done in New Zealand also indicated that the X-ray pattern of DNA is not inconsistent with both types of twists being present in the polynucleotide chain. Such a structure, with alternating right and left-handed helices, was given the name side-by-side structure.

Although the above-mentioned structure had been shown by theory to be very satisfactory and biologically very possible, it received proper attention only when crystallographic structure determination of oligonucleotides actually gave evidence of the left-handed twist being present. In this also, the first clear cut non-Watson-Crick type of twist was shown by Viswamitra from Bangalore. Very soon, left-handed twists themselves were observed by Rich and coworkers at MIT and Dickerson in Caltech. The reason why these specific examples

are cited is because it was only after the experimental observation by crystallography had been made, that the molecular biologists believed the side-by-side structure and worked out its consequences for molecular biology. It is rather interesting that the actual left-handed helix (the so-called Z-helix of Rich) has for its repetition two nucleotide units instead of one. Yathindra from Madras has actually shown that among helices built with two nucleotide units as the repeating structure, the Z-helix is a very good one.

Since our interests are only in molecular biophysics, we shall not comment about various chemical and biological observations that have been made the Z-helix, and the applications that it has found in the field of molecular biology. However, it must be emphasized that the crystallographic structure determinations of the conformations of very big oligonucleotide structures were really the ones that have led to appreciable progress in our knowledge nucleic acid structures during the last five years.

5. Molecular theory of life processes:

The subject of molecular biophysics with special reference to the explanation of biological processes, has grown widely,

and this section can only give a very small number of examples in this field. I have chosen the examples to illustrate different ways in which conformational analysis of biopolymers and related compounds has helped in understanding many features of this type and even led to suggestions of possible modifications of the biosystems.

(a) Collagen primary structure: As mentioned earlier, the triple helix of collagen requires the presence of glycine at every third position, and of proline and hydroxyproline in the locations X and Y, in the sequence -Gly-X-Y- . Of these, a good number of X's are Pro's while most of the Pro's in position Y are hydroxylated to form hydroxyproline (Hyp). The role of Hyp in collagen had not been known at all for a long time. We shall discuss it a little in detail in the next subsection; but now we need only note that hydrogen bonds arising from the OH group of hydroxyproline going via water molecules to neighbouring chains is a very important feature of the collagen structure. It is also a fact that, apart from Gly being at every third position, there is an approximate repetition in the primary structure at a larger interval of about twelve tripeptide sequences. I had always commented on this and indicated that the collagen molecule consisting of about 1000 residues is probably not produced by a single gene, but by repetitive patterns

based on some smaller genetic units. During the last couple of years, studies on the collagen gene has indicated that it is in fact based on such repetitions. The consequence of this for the understanding of the secondary and tertiary folding for the collagen structure have not been yet carried out in good detail. This is an open problem.

(b) Role of hydroxyproline in collagen: As mentioned above, Hyp residues occur only in the position Y and actually the collagen molecule as it is synthesized from messenger RNA contains no Hyp, since only Pro is coded by the genetic code. The enzyme collagen proline hydroxylase adds the OH group to the carbon atom 4 of proline and that too only in the trans configuration. This great specificity of the enzyme is reflected in the fact that only 4-trans Hyp can lead to the stabilising hydrogen bond via water that was mentioned above. In fact, it has been found, by experimental studies, that if procollagen, as it is synthesised first and which does not have Hyp is studied with regard to its triple helix forming property, it is found to have a melting temperature well below the body temperature. However, when Hyp's are formed at points Y, the melting temperature rises to more than 45°C. Thus, the very existence of strong fibres of collagen requires Hyp residues in the proper places.

The occurrence of hydrogen bonds associated with Hyp were derived theoretically in our laboratory in Bangalore by Manju Bansal, R.S. Bhatnagar, and myself. Its verification in relation to melting temperature etc. came from studies carried out at the same time in two different laboratories. Thus collagen prolins hydrolase is a vital enzyme for collagen by synthesis. It has as co-factor ascorbic acid (vitamin C) and this probably explains the occurrence of the collagen disease scurvy of the skin where there is deficiency of this vitamin. However, vitamin C probably has an even more important role. It is known that in the immune response system, immunoglobin attaches itself to the complement C1q which then goes through a series of reactions leading to the destruction of the organisms causing disease to which the immunoglobin had first attached itself. It was a great surprise for me when I learnt that the laboratory of Prof. Porter in Oxford had found, in the sequence of complement C1q, glycine at every third position and both proline and hydroxyproline also being present, just as in collagen, for a good length of its sequences. It is reasonable, therefore, that complement must have the collagen triple helix structure for a good part of its secondary structure. This has been verified by electron microscopy. What is more is that Hyp also occurs in the complement sequence

at the Y position and for it to be produced the proline hydroxylase enzyme is obviously needed and, hence, also the cofactor, vitamin C. Thus the importance of vitamin C for immunity in general is brought to the forefront. A paper on this was published by me in the International Journal of Quantum Chemistry 1978 and may be referred to for more details about this theory.

(c) Enzyme binding the substrate: The first globular protein to be solved were myoglobin and haemoglobin. These are not enzymes, but oxygen-carrying blood proteins. Lysozyme was the first enzyme-like protein to be solved and in this the enzyme substrate binding was beautifully illustrated by X-ray crystallography by Phillips and co-workers. Since then, a very large number of enzymes have been solved by crystallography and the active site has been carefully examined. It is then found that the geometry of the active group as such, which is involved in the substrate binding is practically identical in the same enzyme from different organisms, and this too, inspite of the fact that the primary structure may be widely different, even in length. This has been illustrated in a very striking manner by Dickerson in the Proceedings of the Symposium on Biomolecular Structure, Conformation, Function and Evaluation held in Madras in 1978. He has shown how

cytochrome-C has exactly the same configuration of groups about the heme in spite of the fact that the number of residues varies between 82 and 134 in the different proteins whose crystal structure analysis had been done at that time.

This observation makes it easy to understand the similiarity in specificity of enzyme-like proteins of similar nature, namely that their active sites after folding are geometrically very similar. However, so far no theorist has been able to predict which sequences for a protein would permit the particular active site configuration to be taken up. This is a challenge to theoretical molecular biophysicists.

However, recently Dr. V.S.R. Rao in Bangalore has worked out from conformational theory, the series of conformational changes that take place when an inhibitor enters the active site and gets bound. Such dynamical studies will throw lot of light on enzyme-substrate interactions.

(d) Haemoglobin: The structure of haemoglobin is one that has been most widely studied, including haemoglobin found in certain types of genetic diseases. In particular, sickle cell anemia is produced only by changing a single amino acid Glu 6 to Val 6 in the β-chain of haemoglobin (which, as is well-known, contains two α-chains and two β-chains). X-ray crystallography

of this protein made by Werner Love of Johns Hopkins has indicated that the molecules of sickle cell haemoglobin do not form tetramers (α_L β_L) but rather have a long chain-like association $\alpha\ \beta\ \alpha\ \beta\ \alpha\beta$.... This presumably weakens the ability of the molecule to transport oxygen to the cells. I had the idea that this change in association must be due to the alteration from the polar nature of the side chain in Glu to the hydrophobic non-polar side chain of Val. On discussion with Love it was found that the association found in the crystal structure of sickle cell Hb, which is different from normal Hb, could be explained by this physical property being different in the two cases.

What about a medical relief for this disease? Obviously one must introduce extra polar groups producing hydrogen bonds, and urea as a medicine seems to be suggested. I learn that many doctors prescribe a drink of urea when there an acute crisis in sickle cell anemia; but this is not a very satisfactory solution, since urea is a waste product of the human body. Other small compounds having plenty of OH groups like glyceraldehyde have been suggested; but no definitely satisfactory solution is available for normal use. I wonder whether genetic engineering can help — namely by somehow

introducing normal haemoglobin β-chain genes into the genetic mechanism of the animal. I am not an expert in this field, and this suggestion has been made because I think the evidence is very strong that the sickle cell anemia arises only from the simple change of the sequence GAC for Glu to GCC for Val, and the consequent change of the physical property of residue 6, from a polar to a non-polar nature. Here is an example where such a thing as a pathological condition can be connected to a change in a small number of atoms in one of the biomolecules involved in the normal metabolism.

(e) Mode of action of carcinogens and of drugs that interact with nucleic acids:

We we have seen, nucleic acids form a double helix with the planar bases of each nucleotide unit leading to hydrogen bonds between the two chains at regular intervals. The standard distance between two such bases stacked one over the other is about 3.4 Å . It is well-known that many aromatic multicyclic organic compounds can produce cancer. That they interact with DNA is known and one of the possible explanations that may be given is that they go and orient themselves in between two stacked base pairs, which is possible because

the bases themselves are also aromatic and π-electron bonds greatly stabilize such a molecular arrangement.

On the other hand, the same process of planar aromatic molecules entering and stacking themselves in between base pairs can be used to stop the reproduction of DNA and thus inhibit cell reproduction, which makes such molecules behave as antibiotics.

In both these cases, the main physical principle is the formation of π-electron bonds which make the aromatic planar molecules arrange themselves in between successive DNA base pairs. For a long time, this was only a theoretical idea, but in recent years, a series of brilliant X-ray crystallographic studies have been made by Sobell and they have clearly shown that the interaction between the aromatic molecules and DNA is exactly what is mentioned above. The still more detailed information of exact atomic positions in the stacking arrangement will lead to the design of drugs having various types of specific biochemical properties. (Incidentally, perhaps the largest population of Indian crystallographers in any laboratory in USA is to be found with Sobell.)

(f) Antibiotics like penicillin: In general, all antibiotics inhibit some biological activity in cells, and they often

preferentially affect more rapidly growing organisms like invading bacteria than the cells in tissues. However, the mode of action of antibiotics are so varied, that a general discussion is not possible. We shall consider one example, namely the mode of action of the penicillin group (β-lactam antibiotics), which actually prevent the formation of the cell wall in bacteria by inhibiting the enzyme that builds the pentapeptide chain between two neighbouring polysaccharide chains in the cell wall. As a result, cell wall is not properly formed and the pathological organism does not multiply. It is interesting that a very satisfactory theoretical explanation, based upon a detailed conformational analysis, has been made by V.S.R. Rao in Bangalore, which explains the imitation by the D-L amino acid sequence in penicillin of the —D Ala —D Ala sequence of the bacterial cell wall pentapeptide. This explanation is beautiful, when one examines the molecular shapes of the enzyme substrate and the inhibiting compound — namely penicillin —which are chemically very different, one being an LD sequence, while the other is DD.

Thus, it will be seen that many facets of activity and properties of biological systems can be explained by examining the properties of the three-dimensional stereochemistry of the molecules that go to constitute them and by studying their nature, both by theory and, in particular, by X-ray crystallographi techniques.

IMPOSSIBILITY OF PARADOXES AND INCOMPLETENESS IN LOGIC*

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Matphil Reports No. 30
March 1983

*for private circulation only

SUMMARY

This paper is an attempt to deduce interesting and valuable conclusions from our vector-matrix Boolean algebraic representation for logic in general. From the isomorphism between Boolean algebra of genus n (BA-n) and n-valued logic (L_n) obtained via the theory of relations where only two states of existence are envisaged for a relation (namely 'yes' and 'no', represented by 1 and 0 respectively in BA-1), it is shown that the completeness of Boolean algebras demand completeness of all L_n (n finite). Similarly, paradoxes occurring in 2-valued L_2 (propositional calculus (PC) represented by BA-1), are all shown to lead to the third and fourth states of BA-2, required by the extended form of PC, namely Syād-Nyāya-System (SNS), and perfectly defined and permitted by this formulation of PC. The examples of the Cretan Liar Paradox (and the generalization of this, namely Double-Statement Paradox), Cantor's Paradox and Russell's Paradox are examined and shown to be amenable to this treatment. Also, Gödel's incompleteness theorem is seen to be

taken care of by formulating quantified predicate logic (QLP) in its extended form (EQPL) isomorphous to BA-3, so that EQLP is as complete as PC in SNS form. However, all finite BA-n have an element of incompleteness in them, in that they lead to a higher genus BA-m ($m > n$) successively, going on to $n = \infty$.

Impossibility of Paradoxes and Incompleteness in Logic

CONTENTS

1. Introduction

As is well-known, "Logic" is the "Science of Reasoning". Therefore, it is self-evident that logic cannot be defective, in that it contains within itself possibilities like the occurrence of a "paradox" (see Section 2 for a definition), in some formulation of it being "incomplete" (see Section 4 for the definition of "completeness"). In the accepted formulations of Propositional Calculus (PC), and of Quantified Predicate Logic (QPL), one or the other of these occurs inevitably, and there is no explanation as to why such possibilities do not violate the validity of the whole system of axioms or assumptions (postulates), which form the basis of the particular branch of logic.

In this paper, we show that "logic" (including PC and QPL as particular sub-systems of it) is perfect, and that the

imperfections of the above types can be eliminated — e.g. for PC, by expanding the set of postulates to obtain the "extended propositional calculus" (Syad-Nyaya System, SNS, see [1]), and for QPL by extending it to the "extended predicate calculus" (EQPL, see [2]). The type of extension, which is adopted for PC and QPL, is also applicable to all multi-valued logics in general, and thus eliminates any possible incompleteness or paradoxical situations.

Necessarily, since the whole approach is novel, the treatment given in the present paper employs the terminology and symbology of References [1] and [2], and we also assume the formulation of the outline of the General Theory of Relations, along with the Boolean Algebraic (BA) representation of this, as developed in [2].

b) Isomorphism between BA-n and n-valued logic

The isomorphism between Boolean algebras of genus n (BA-n) and multi-valued (n-valued) logic (L_n) has been shown to be present [2], provided the right choice is made of the corresponding entities in BA-n and L_n (namely Boolean vectors ≡ terms, and Boolean connectives ≡ logical connectives) However, the two-valued logic (L_2) of Propositional Calculus (PC) is conventionally represented by BA-1 having only one state (T) and its negation (F). By making a careful analysis of the operators that occur in BA-n, it has been shown [1] that L_2 is much better represented by BA-2, having four truth values "true" (T), "false" (F), "doubtful" (D) and "impossible" (X), in order to cover its full consequences, rather than by BA-1. The BA-1 representation is isomorphous to a sub-algebra of BA-2 and it can represent only the states having the truth values T and F. This algebra necessarily gives rise to the states

D and X given by $T \oplus F$ and $T \otimes F$ respectively — in addition to the states T and F of PC. We call the BA-2 implementation of PC as SNS, standing for Syād-Nyāya System (Syād = may be; Nyāya = logic in Sanskrit).

As will be shown below, one of the consequences of this BA-2 representation of L_2 is that the famous paradox arising from the statement of the "Cretan Liar" (who says, in effect, "What I say is false") is eliminated, and the statement can have one of the available states D or X of BA-2. The above sentence of ours will look very puzzling in the form it is now given; but it will be clarified as we go on to Section 2. The point we wish to emphasize is that, by suitably augmenting the structure of the logic used, and the associated Boolean algebra, we can effectively modify what appears to be a paradox, into something that is a perfectly permissible statement in a higher logic, whose acceptability is shown by its isomorphism to some higher BA-n.

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As regards "incompleteness", this occurs, for instance, in the standard treatments of QPL, using the states "for all" ($\forall$) and "there exists" ($\exists$), whose complement is "for none" ($\nexists$). Thus Godel's incompleteness theorem, put in our language, says, in effect, that "In any theory based on first order predicate logic, there are statements, derivable from a finite set of "axioms", which can neither be proved to be true nor proved to be false". We shall show (in Section 4) that, if QPL is made complete by extension to EPL, by means of an isomorphism to BA-3, then this formulation has a third basic state, Σ, which has just this property — "sometimes true, but not always true, or always false"— and a set of statements using only $\forall$ and $\nexists$ and their negations, Λ and $\exists$ (see [2] for notation of QPL and EQPL) can always be constructed to lead to the state Σ, which is a perfectly admissible state in BA-3, and makes it "complete" (in the usual sense it is used for PC).

We shall discuss paradoxes and their resolution, in some detail in Sections 2 and 3.

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2. Discussion about paradoxes

(a) Genesis of a paradox in classical logic

A paradox arises when two resultant states for a statement in an argument are mutually contradictory, and this contradiction is inescapable. Thus, an argument, starting from one or more input statements, may lead to two different states $\underline{\underline{s}}_1$ and $\underline{\underline{s}}_2$ for a sentence derived from them, which are such that

$$\underline{\underline{s}}_1 \underline{\underline{V}} \underline{\underline{s}}_2 = (0 \quad 0) = X \text{ (Contradiction)} \qquad (1)$$

Since, according to classical logic, this occurs only if one of $\underline{\underline{s}}_1$ or $\underline{\underline{s}}_2$ is T and the other is F, then either $\underline{\underline{s}}_1$ or $\underline{\underline{s}}_2$ must be negated, in order to avoid the contradiction. This leads to

$$\text{Either} \quad \underline{\underline{s}}'_1 = \neg \underline{\underline{s}}_1 \quad (a) \quad \text{or} \quad \underline{\underline{s}}'_2 = \neg \underline{\underline{s}}_2 \quad (b) \qquad (2)$$

If we now put in $\underline{\underline{s}}'_1$ (or $\underline{\underline{s}}'_2$, as the case may be) into the argument, we can work backwards all the steps of the argument

by reversing the logical steps present originally in it.

Then, one of three possibilities can occur:

(a) Some input term(s) or sentence(s) arising from the changing of $\underline{s}_1$ to $\underline{s}_1'$ has to be negated (3a)

(b) Similarly, the argument reversed from $\underline{s}_2'$ leads to some input(s) being negated (3b)

or

(c) Some logical step(s) in the argument (composed of one or more statements) have to be changed and restated so as to be consistent with $\underline{s}_1'$ (or $\underline{s}_2'$, as the case may be). (3c)

Putting these in a nutshell, a contradiction X at one stage of an argument demands a change in the classical state T or F of one or more statements which have been put in as inputs; or the argument itself is defective.

It may happen, as we will show in connection with some well-known paradoxes (see Section 3) that none of (3a), (3b),

(3c) becomes possible, in some examples. In other words, the argument is well formulated, the inputs are all correct, and yet we get out of the whole argument two terms, or sentences, $\underline{\underline{s}}_1$ and $\underline{\underline{s}}_2$, which are mutually contradictory, as shown by the emergence of the contradictory state X. When one of $\underline{\underline{s}}_1$ is made $\underline{\underline{s}}_1 \underset{\sim}{N} = \underline{\underline{s}}_1'$ (or $\underline{\underline{s}}_2 \underset{\sim}{N}$ is made $\underline{\underline{s}}_2'$) and the argument reversed, it leads <u>again</u> to a <u>contradiction</u>. In such circumstances, we have a paradox. (Incidentally, even if one of $\underline{\underline{s}}_1$, or $\underline{\underline{s}}_2$ is itself an <u>input</u>, and the other is a deduced <u>output</u> from the argument, and Eqn. (1) holds, all that have been mentioned in (2) and (3) and their consequences are still applicable.) Thus. <u>a paradox is a contradiction that cannot be eliminated</u>.

We shall give in the next subsection (b) some well-known examples of such paradoxes. In order to see how we dissolve them away, we shall consider examples of arguments, in which

a contradiction leads to a useful conclusion, and it will be seen that what happens is that one of (3a), (3b), (3c) is employed for this purpose. Therefore, it seems reasonable that, even in the case of an (apparent) paradox, the solution is to make one of (3a, b, c) operative, by making the logic to be of a higher genus (i.e. isomorphous to a higher genus BA), e.g. going from BA-1 to BA-2 ($\equiv$ SNS) for classical logic. This is considered in Section 3.

(b) Typical examples of paradoxes

We shall now consider two well-known paradoxes — the Cretain Liar Paradox (CRLP) and Cantor's Paradox (CNTP) and put them in our notation, so as to verify how they stand in relation to the conditions (3a, b, c). (No references are given, as these are well-known).

In CRLP, a Cretain says that "All Cretans are liars"; and the question is — "Is what he is saying true or false?"

We shall discuss it in a slightly modified form by the Cretan liar saying, in effect,

CRLP: "If whatever I say is false, is the statement asserted by me now true or false?" (4)

Curry's paradox is:

CNTP: "Does the set of all sets contain itself or not?" (5)

In the former case, the answer is "T, F, T, F, . . . ", in endless succession, while the latter leads to both "yes" and "no". The paradox lies in the fact that no definite state T or F (the only ones available in CL) is possible for the statement under consideration.

Before analyzing the above two examples of paradoxes, we shall consider a pair of statements made by two different persons A and B, which can also lead to a situation very similar to that for CRLP in that a term has an endless succession of states "T, F, T, F. . .". We call this the Double Statement Paradox (DBSP), and it is as follows:

Double Statement Paradox

(i) A says (a) ≡ "What B says (b) is false". (6a)

and

(ii) B says (b) ≡ "What A says (a) is true". (6b)

Here, it is readily verified that, irrespective of a being T or F, successive applications of (i) and (ii) gives the states T, F, T, F, . . . for the statement a (and similarly for b also). We shall consider the solution of the DBSP first in the Section 3(c), when it will become apparent that CRLP is a particular case of DBSP, when the two persons A and B are one and the same (See Figs. 2(a) and (b) therein.) The logical feature that is common to Cantor's paradox and the Cretan Liar paradox will also be considered there, as also a variant of Cantor's paradox known as Russell's Paradox (RSLP). CRLP typifies a whole series of paradoxes, for which we shall indicate a common solution in Section 3.

(c) Aetiology of a typical contradiction, which leads to a paradox

We have considered the genesis of a paradox in the last sub-section and seen that it is intimately connected with the occurrence of a contradiction, and the attempt at resolving the contradiction being unsuccessful. Hence, in order to study a paradox quite completely, it is necessary to know the aetiology of contradictions. We shall now consider some common types of conditions under which contradictions can arise in an argument. Also, we shall consider briefly, in each case, how the contradiction can be "got over". In case the contradiction can be avoided, this can arise only from some change in the rest of the argument and this will normally give useful information. Obviously, when such a change cannot be carried out, we are in trouble and come at an impasse; and there is a paradox. Our contention is that the impasse occurs only when states existing in pure classical logic alone are

employed; but that it can be dissolved away, if states existing in other higher ~~order~~ genus logics with equivalent Boolean algebras of higher genus are utilized, as in SNS logic for CL.

We shall now consider the essential structure of an argument that leads to a contradiction, and discuss some examples. These are not necessarily a complete set, but representative enough for our purpose.

Case (i): Two paths from a single assumption to a single conclusion

Suppose we start from an input ($\underline{a}$) and go via two different paths and arrive at the states $\langle b_1|$ and $\langle b_2|$ of the term $\underline{b}$. Then, it is sometimes possible that these two states are T and F; or F and T. In either case,

$$\underline{b} = \langle b_1| \vee | b_2\rangle = \langle X| \qquad (7)$$

It is impossible to get over this contradiction, if the essence of the relation between $\underline{a}$ and $\underline{b}_1$, and between $\underline{a}$ and $\underline{b}_2$, are as in 8(a) and (b):

$$\langle a \mid \Sigma \mid = \langle b_1 \mid^{(a)}; \quad \langle a \mid N \mid = \langle b_2 \mid \quad (b) \qquad (8)$$

In such a case, if the CL state of $\underline{b}$ is negated we obtain either (9a) or (9b).

$$\langle b_1 \mid N \mid = \langle b_1' \mid \quad (a) \quad \text{or} \quad \langle b_2 \mid N \mid = \langle b_2' \mid \quad (b) \qquad (9)$$

If now, the argument is reversed from $\underline{b}_1'$ and $\underline{b}_2'$ towards $\underline{a}$ to give $\langle a_1' \mid$ and $\langle a_2' \mid$, then, necessarily, from the appropriate reverses of (8), we obtain,

$$\langle b_1' \mid N \mid = \langle a_1' \mid = \langle a \mid N \mid ; \quad \langle b_2' \mid N \mid = \langle a_2' \mid = \langle a \mid \qquad (10a)$$

or

$$\langle b_1 \mid \quad \mid = \langle a_1' \mid = \langle a \mid ; \quad \langle b_2' \mid N \mid = \langle a \mid N \mid = \langle a_2' \mid \qquad (10b)$$

In either of the cases (10a) or (10b),

$$\underline{a}' = \langle a_1' \mid V \mid a_2' \rangle = \langle a \mid N \mid V \mid a \rangle = \langle X \mid \qquad (11a)$$

or

$$\underline{a}' = \langle a' \mid V \mid a' \rangle = \langle a \mid V \mid N \mid a \rangle = \langle X \mid \qquad (11b)$$

In other words, what was a contradiction between the states

$\underline{b}_1$ and $\underline{b}_2$ in (7) becomes now a contradiction between the two possible states for $\underline{a}$ that we get from the revised states of $\underline{b}$ and coming back <u>via</u> the same two (different) paths to $\underline{a}$.

This is a symbolic example of a typical "paradox", and as we will see in Section 3, it contains the essential features of CRLP, CNTP and a third one discussed therein "Russell's paradox" (RSLP). In this, what we use in effect to prove the paradox is the well-known theorem in Classical Propositional Calculus (see [4] p. 187) which can be stated as follows:

<u>Theorem 1</u>

If an argument based on well-formed formulae and an input $\underline{a}$ leads to an output $\underline{b}$, which is either T or F, but in contradiction with the known state of $\underline{b}$, then it follows that the same well-formed formulae, with $\langle b|$ replaced by $\langle b'| = \langle b\,|\,N|$, will inevocably lead to the state $\langle a\,|\,N|$ for $\underline{a}$. (This is the essence of the <u>reductio ad absurdum</u> proof).

In our case (i), this ~~formulae~~ theorem has been applied for each of the two different paths by which we go from $\langle a|$ to $\langle b_1|$ and from $\langle a|$ to $\langle b_2|$. Clearly, either of the $\underline{b}$'s has to be negated so as to obtain consistency between $\langle b_1|$ and $\langle b_2|$. Then, if the effective relations between $\underline{a}$ and $\underline{b}$ are 8(a) and (b), then immediately we get inconsistency between $\langle a_1'|$ and $\langle a_2'|$ generated back <u>via</u> <u>the same two paths</u> from a common $\underline{b}$; and the contradiction is in the form of Eqn. (11a) or (11b). Hence, if the logic of the argument is completely foolproof and unquestionable, then the set of statements under consideration forms a paradox.

We shall associate the structure of this general paradox with that of the particular classical examples like $C^{R}_{\$}LP$, CNTP and RSLP in Section 3. We shall show how the paradox can be resolved by using SNS logic for this typical contradiction

(Case (i)) in Subsection 2(d). It is very simple, but requires only that the states of BA-2 are also incorporated. (We shall also examine Case (ii) and Case (iii) in subsections (e) and (f)).

(d) Argument of Case (i) treated in SN3 logic

In CL, there are only two states T and F, and if the same term, or sentence, is found to be both T and F, then it is considered to be a contradiction. In SNS, isomorphous to BA-2, T is equivalent to (1 0) and F to (0 1), and the state T "and" F, (which is really $T \otimes F$), is the contradictory state (0 0), obtained as in (12a).

$$T \otimes F = (1\ 0) \otimes (0\ 1) = (0\ 0) = X \qquad (12a)$$

However, there is a fourth state, T "or" F ($T \oplus F$), which can be considered when $\langle a_1|$ and $\langle a_2|$ are T and F respectively. It is not an "impossible" state, but it is the "doubtful" state,

as in (12b):

$$T \oplus F = (1 \quad 0) \oplus (0 \quad 1) = (1 \quad 1) = D \qquad (12b)$$

If, now, we take this D to be state of $\underline{b}$, arising from $\underline{b}_1$ and $\underline{b}_2$ — viz. $\underline{b} = \underline{b}_1 \oplus \underline{b}_2$, then it means the following: "The state of $\underline{b}$ <u>may be</u> true or false; and, in the absence of further information, we cannot decide between the two". What is even more interesting is that, if the state D is put for both $\underline{b}_1$ and $\underline{b}_2$ and the argument is reversed, with $\langle b_1' | = D$, $\langle b_2' | = D$, we obtain $\langle a_1' | = D$ and $\langle a_2' | = D$ and $\underline{a} = \langle a_1' | \; V \; | a_2' \rangle = D$ (with no contradiction). Thus, $\underline{a} = D$, $\underline{b} = D$ is a <u>permissible solution in</u> SNS for paths of the type used in the DBSP, and their reversals. /// The proof that $\langle a_D | \; N | = \langle a_D |$ follows from $|N| = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ in SNS logic. In essence, it is based on the simple result that $\langle a_T | \rightarrow \langle b_F |$ and $\langle a_F | \rightarrow \langle b_T |$ when $\underline{a}$ is "negated" to $\underline{b}$. Hence, $a_T \oplus a_F = a_D$ on negation becomes $a_F \oplus a_T$ which is also equal to a_D, since the operator $\oplus$ is commutative. 2

(e) Case (ii) of contradictions and analogy to CRLP & CNTP

The special case of case (i) of an argument, going from an input $\underline{\underline{a}}$ to two outputs $\underline{\underline{b}}_1$ and $\underline{\underline{b}}_2$ via two different paths, can be made even shorter, by $\underline{\underline{a}}$ being connected to $\underline{\underline{a}}$ itself via some argument. We shall take the simplest of these, namely,

$$\text{Case (ii)} : \quad \underline{\underline{a}} \Longleftrightarrow \neg\, \underline{\underline{a}} \tag{13}$$

Here, if we designate the input state $\langle a_1|$ by $\underline{\underline{a}}_1$ and the output state $\langle a_2|$ by $\underline{\underline{a}}_2$, we have the following two possibilities in CL:

$$\langle a_1| = T\,, \quad \langle a_2| = F\,, \quad \langle a_1| \underset{\sim}{\vee} |a_2\rangle = \underline{\underline{a}}_1 \otimes \underline{\underline{a}}_2 = X \tag{14a}$$

or

$$\langle a_1| = F\,, \quad \langle a_2| = T\,, \quad \underline{\underline{a}}_1 \circledast \underline{\underline{a}}_2 = X \tag{14b}$$

and we get a paradox, since both $\underline{\underline{a}} = T$ and $\underline{\underline{a}} = F$ lead to a contradiction. This is perhaps the simplest of paradoxes in

symbols (characterising a whole species, of which the CRLP is a particular example).

However, the moment we work in SNS logic, we have the third possibility of states for (13), viz:

$$\langle a_1| = D \; ; \quad \langle a_2| = D\,\underset{\sim}{N} = (1 \quad 1)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = (1 \quad 1) = D \qquad (14c)$$

so that

$$\langle a_1|\, V \,|a_2\rangle = D \circledast D = (1 \quad 1) = D \qquad (14d)$$

and there is no contradiction. Hence the equivalence in (13) is satisfied by $a = D$, and this means that we are unable to assert whether $\underline{a} = T$ or $\underline{a} = F$.

A fourth possibility is there for $\underline{a}$ satisfying the equivalence (13), namely $\underline{a} = X$, since

$$\underline{a}\,\underset{\sim}{N} = X\,\underset{\sim}{N} = (0 \quad 0)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = (0 \quad 0) = X = \underline{a} \qquad (15)$$

Hence, the paradoxical equivalence (13) for $\underline{a}$, in CL, is a w.f.f in SNS, with $\underline{a}$ having the state of, either "doubtful

truth or falsehood", or of "impossibility". In the case of CNTP, we see straightaway that X is a possibility — i.e. there exists no "Set of all sets", just as "There is no last integer" (as in Peano's axioms for integers). The other possibility is that of D, viz. that the "Set of all sets" (which is infinite) both contains itself and does not contain itself, just like infinity is both equal to itself and not equal to itself (see Section 3 for more details). In the CRLP also, the solution is that the statement made by the person is invalid, or "impossible" (X). There is also a second possibility (namely D), which gives no information content to the statement of the Cretan Liar, although it is not impossible. We know nothing more about the credibility of the Cretan than before we heard his strange sentence (See Section 3).

(f) Case (iii) and analogy to DBSP

This is similar to case (i), but differs in that there are

two statements in two variables in a circuit ($\underline{a} \overset{E}{\longmapsto} \underline{b} \overset{N}{\longmapsto} \underline{a}$):

$$\underline{a} \Longleftrightarrow \underline{b} \quad \text{(a)}; \qquad \underline{b} \Longleftrightarrow \neg \underline{a} \quad \text{(b)} \tag{16}$$

By putting (16b) after (16a) we obtain

$$\underline{a} \Longleftrightarrow \neg \underline{a} \; ; \quad \text{contradiction in CL} \tag{17a}$$

and by putting (16a) after (16b), we obtain

$$\underline{b} \Longleftrightarrow \neg \underline{b} \; ; \quad \text{also a contradiction in CL} \tag{17b}$$

Hence, 16(a) and (b) together lead to a paradox in CL. However, here again, if SNS is invoked, we can have both $\underline{a} = D$, and $\underline{b} = D$ as a solution for the two Eqns (16a & b). Similarly, both $\underline{a}$ and $\underline{b}$ can be equal to X.

Any number of examples of arguments can be built up, for which neither the state T nor the state F is possible for a number of inputs (outputs), the other inputs, outputs and the sentences of the argument being specified. Since they do not exemplify any new ideas, we shall not discuss them here.

3. Resolution of actual examples of paradoxes

In the previous section, we had shown how the introduction of the states D and X leads to a method of getting over the paradoxical situation — namely that an argument leads to a contradiction, and when this contradiction is removed and the argument traced back, it leads to another contradiction against the assumption(s). In all the three cases (i), (ii) and (iii) considered in the last section, the essence of the contradiction is that $\underline{a} \otimes \neg \underline{a}$ is found to occur, which, in classical logic, is a contradiction. However, if the state D (of SNS logic) is permitted, then $\neg \underline{a} \Longleftrightarrow \underline{a}$ and $\underline{a} \otimes \neg \underline{a}$ is not a contradiction. The state a_D, when negated, gives once again the state a_D identical with itself, and we have only to say that the statement under consideration cannot be proved to be either true, or false. Such a situation is not considered as being illogical in SNS (and also in QPL, as we will show later).

To bring the whole argument into the forefront, we may say that the essentially contradictory situation that exists in all paradoxes — namely that $\underline{a} \underset{\sim}{\vee} (\underline{a}\ N) \neq \underline{x}$ (= X) is a contradiction in CL (with only T and F as the allowed states) — has a permitted state in SNS logic — namely the state D = (1 1) for both $\underline{a}$ and $\underline{a}$ N, in which case $\underline{x} \neq X$. Boolean algebra permits this state D, and its corresponding logical analogue is best put as follows: "The term $\underline{a}$ may be true or may not be true; we cannot decide between the two, with the conditions given in the problem".

In order to indicate how such possibilities, namely <u>being both true and false at the same time</u> occurs in real arguments, we shall take an even simpler example than the "Set of all sets" which was considered in the previous section. We shall consider the integer $\infty 0$, and show that some properties of integers (which can only <u>either</u> exist (T) <u>or</u> not exist (F) for finite

integers) assume the state D when the integer becomes infinite. In fact, it is well-known in pure mathematics that an infinite set is that which can be put in one-to-one correspondence with a subset of itself, an operation which is impossible for any finite set.

- <u>(a) Paradoxical properties of infinity</u>

This sub-section will be written in an intuitive manner without very rigorous arguments, since it is intended to be illustrative, rather than being used for proving any theorems related to infinity. Thus, given two finite numbers m and n, we can always ask the question — Is m equal to n $(m = n)$ or not? If $m \neq n$, obviously $m \gtrless n$. Thus, we have the two mutually exclusive states $\underline{a}$ and $\underline{b}$, as in (18):

$$a \equiv (m = n), \qquad b \equiv (m \gtrless n) \tag{18}$$

The two equations in (18) represented by the terms $\underline{a}$ and $\underline{b}$

have the logical properties expressed by (19a) and (19b).

$$\underline{a} = \neg\, \underline{b} \quad (a) \; ; \qquad \underline{b} = \neg\, \underline{a} \quad (b) \qquad\qquad (19)$$

Eqns (18) and (19) are completely true for any finite integer and also for any finite number (positive numbers only will be considered here for convenience). It is well-known that infinity has properties rather strange and different from ordinary numbers. Quoting for instance from Bertrand Russell's book "Mathematical Philosophy" [5], we find on page 86, the equation

$$\alpha = \alpha + 1$$

If we take any finite number n , then the equation $n = n + 1$ is absurd and is contradictory by Eqns (18) and (19). The method of proving the contradiction can be put very simply as follows. If $m = n + 1$, then $m > n$, so that $m \neq n$ ($\underline{b}$ say)

On the other hand, (20) leads, in the finite case, to

to $m = n$ ($\underline{a}$ say), and clearly $\underline{a}$ contradicts $\underline{b}$, if

n is finite.

Yet it is well-known that the theory of infinity demands many equations of the type (20) and they are all taken to be completely valid in spite of the above logical contradiction that we have indicated, for all finite n. The explanation given (for the absence of contradiction) is to say that the properties of infinity are different from the properties of finite numbers. Thus, if we take the property of equality and inequality of numbers, these two are mutually opposed, or contradictory to one another, for finite numbers; but that both can be true for infinite numbers. In other words, if a number is infinite, then it "may or may not be" equal to itself. Both the results

$$m = n \quad (a) \quad \text{and} \quad m \neq n \ (= m + 1) \quad (b) \qquad (21)$$

can be proved (with $m = \infty$, $n = \infty$), according to the particular

circumstance of the problem concerned. In SNS logic, we will say that the Eqns. (21a and b) will make the number infinity have the SNS state D, for the property of equality between m ($= \infty$) and n ($= \infty$). Thus, without going into any classical paradox, but only considering the properties of infinity (completely as it is understood by pure mathematicians such as number theorists, function analysts etc.), we can understand not only the nature of the state D of SNS logic, but also the absolute necessity of this in mathematics (See [1] for an explanation of D occurring in very simple logical arguments).

It should be mentioned that the main purpose of our argument in this section is to show that the contradictory equations that are produced from putting $\underline{a} \Longleftrightarrow \underline{b}$ in (19) need not always lead to the state X (contradiction), for it can also lead usefully to the state D, as in the definition of infinity given

in Russell's book, as in Eqn. (20). If this is clearly kept in mind, the explanations that we give below for the resolution of the classical paradoxes, will become quite clear.

(b) Attempt at removing all paradoxes in propositional calculus

As already mentioned, the exact point of the genesis of a paradox in propositional calculus arises from the production of a contradiction from the simultaneous assertion of two contradictory statements — namely

$\underline{a}$ is true (a); $\underline{a}$ is not true (false) (b) (22)

We must note that the pair of statements in (22a) and (22b) themselves need not be contradictory (as mentioned in the previous section) for the states D and X of $\underline{a}$. If the two assertions (22a) and (22b) are irrevocable and no modification can be made in them by looking back into the argument, then a

reconciliation of the two statements can be done within the realm of SNS logic. Thus, if $\underline{a}$ = D (or X), then $\underline{a} = \neg\underline{a}$. Thus, there are two ways open to us for treating a paradox which can be put as follows:

> The statement $\underline{a}$ is doubtful — "may be true or false" — and further information is needed to resolve this doubt and get a clear statement of its being either true or false, (23a)

or

> The statement $\underline{a}$ is invalid and does not relate to a truly existing object. (23b)

The question whether (23a) or (23b) is the resolution of the paradox (22) is not within the realm of logic alone. It depends on the semantics of the subject under consideration. Sometimes invalidity is the right answer, and sometimes impossibility of precise knowledge may be the answer. However,

The real point at issue is that there is no paradox as such, it is achieved by affixing to the statement $\underline{a} = \sim / \underline{a}$. This can be achieved by affixing to the statement $\underline{a}$ one of the SNS states D or X. What leads to a paradox in CL (i.e. neither T nor F) leads one to a possible state (D) in SNS.

In view of what has been stated earlier, the checking of the contradiction (22) backwards to trace its origin need not be done, especially because it is a standard procedure used in the method of reductio ad absurdum. If the argument that led to the contradiction (22) is not water-tight, then such a tracing can be done and something useful and sensible could be derived about one or more of the assumptions (inputs) put into the argument. This is within the realm of ordinary logic and does not belong to the realm of paradoxes. Consequently nothing more is said about this.

(c) Some specific examples from the literature

In all examples, one or the other of the following two possibilities occur — (i) A circular argument leads to

$$\underline{a}\ (=\underline{a}') \ = \ \neg\, \underline{a}\ (= a'') \qquad (24a)$$

(ii) Two ways of interpreting the statements made lead to

$$\underline{a}' \ = \ T \quad \text{and} \quad \underline{a}'' \ = \ F \qquad (24b)$$

The paradox arises from the contradiction $\underline{a}' \otimes \underline{a}'' = X$, although the rest of the argument is correct.

Three practical examples will illustrate these, and we shall indicate how the method of removing the paradox (mentioned in Section 3(b)) works in each case. The first is taken from the article by J.G. Kennedy "Semantics in Logic" in the Encyclopedia Britannica [6] :

The previous sentence ($\underline{a}$) is true; (25a)

The next sentence ($\underline{b}$) is false. (25b)

These correspond completely to the pair (16a) and (16b) dealing with DBSP, and lead to the paradoxical results $\underline{a} \iff \neg \underline{a}$ and $\underline{b} \iff \neg \underline{b}$. The solution is simply that both $\underline{a}$ and $\underline{b}$ are either X or D — i.e. they are invalid sentences (X), or they both refer to something which may be true or false (D). The logical graph of this is shown in Fig. 1(a) (b).

Fig. 1(a) and (b): Two ways of checking the circuit in the logical graph of DBSP. In both cases, $\underline{a} = \underline{b} = D$ is a solution.

Fig. 2.(a): The auto-circuit of $\underline{a}\ \underset{\sim}{N} = \underline{a}$.
(b): Logical graph of checking for contradiction.

The second example is the Cretan Liar Paradox, in which the two statements $\underline{a}$ and $\underline{b}$ are made one and the same. No more need be said, except that $\underline{a}' \underset{\sim}{V} \underline{a}'' \neq X$, if $\underline{a}' = \underline{a}'' = D$. (on Fig. 2).

The third example is Russell's paradox, which comes under

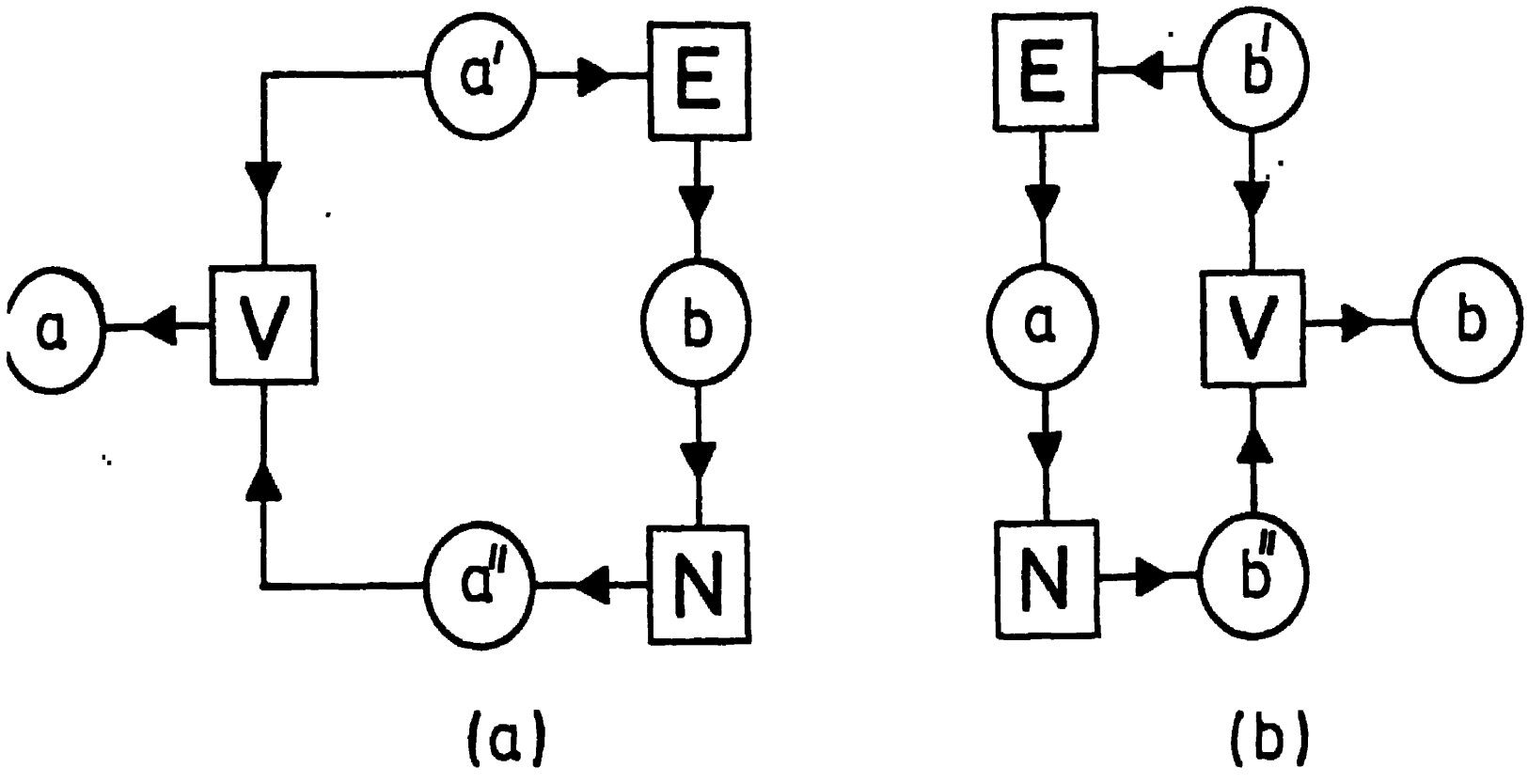

Fig.1

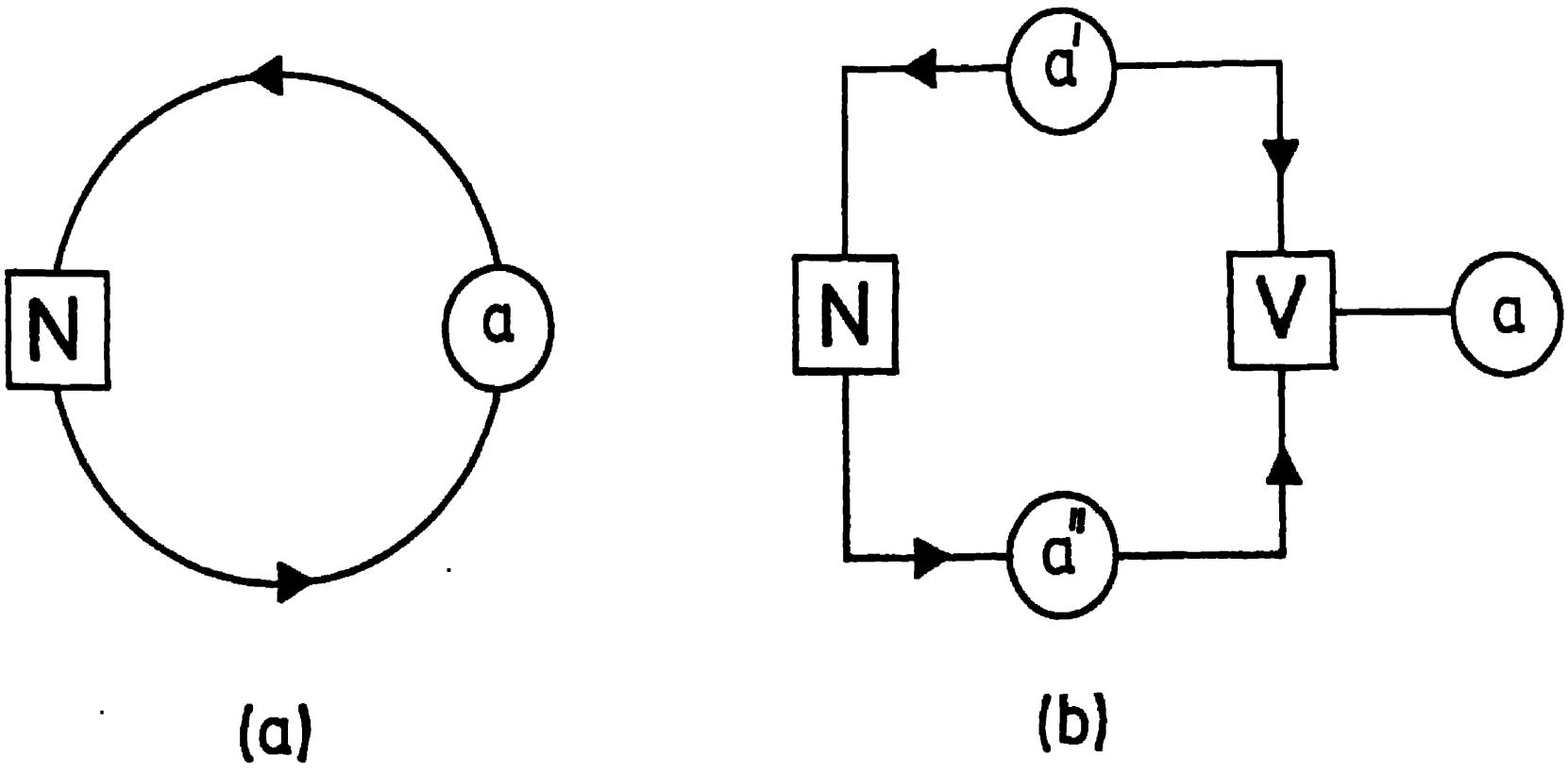

Fig.2

the category (ii) of (24b). The actual one in the literature is slightly different from (5). It is best described by the elegant quotation from the short article on "antinomy" in Encyclopedia Britannica [7]:

> "The line of argument runs: Given any class of things, c for example, either c is a member of itself, or else not—one or the other, but not both. (Thus if c is the class of men, c is not a member of c, since the class of men is not a man; while if c is the class of all classes, c is a member of c, since the class of all classes is itself a class.) Let a class that is not a member of itself be called an exclusive class. Consider (26)
> the class of all exclusive classes, K for example. The object is to determine whether K itself is exclusive or not. If K is exclusive, it has to be a member of K (since K was defined as the class of all exclusive classes). But exclusive means: not a member of itself. So K has to be not exclusive. Suppose, then, that K is not exclusive. This means it is a member of itself. But all the members of K are exclusive classes. Hence, K is exclusive. It would seem, then, that K can be neither exclusive nor nonexclusive, though every class must be one or the other".

It is seen that in RSLP one way of interpreting (26) says the answer is "yes", and another way says it is "no". The emphasis is on "class of all..." for the former, and on "exclusive" for the latter. It is obvious that K is not a finite set, and simple argument shows that this type of paradox cannot be constructed with finite sets. The simultaneous occurrence of contradictory properties for K arises only because it is infinite, and is of semantic origin because of the properties of K that have been invoked. As we have already seen, infinity has properties that are mutually exclusive for finite numbers.

In fact, there are other paradoxes, not involving infinity, in which A has both the properties $\underline{a}$ and $\neg\underline{a}$; but it is the sentence describing it that invokes this strange situation. It is not a logical consequence at all that $\underline{a} \iff \neg\underline{a}$, but both are asserted in the sentence. However, in SNS logic, even this is permissible, and we can say that either A is "impossible" (X) or A "can both have the property $\underline{a}$ and not have it"(D). The ways of using these solutions to such paradoxical definitions have still to be worked out further.

4. Incompleteness of logics examined

(a) The existence of incompleteness in SNS logic:

It is commonly asserted in orthodox theories of logic that propositional calculus is complete, while quantified predicate logic is necessarily incomplete. Put in simple language, the incompleteness of QPL is equivalent to the following statement:

> "Starting from well-known postulates of QPL, one can construct a set of statements which effectively assert that a statement $\mathcal{Q}$ is neither always true nor always false". (27)

In other words, the incompleteness is asserted from the existence of the property (28) for some QPL statement $\mathcal{Q}$.

> " $\mathcal{Q}$ can neither be shown to be always valid nor never valid" (28)

However, in terms of our definitions of the extended QPL states

[2], this is equivalent to saying that

"It is possible for Q to have the EPL state Σ = (0 1 0)" (29)

It is to be noted that (29) is a puzzle in QPL, but completely natural in EQPL, which has the three basic states of BA-3, via (1 0 0) ($\equiv$ for all), (0 1 0) ($\exists$ for some), (0 0 1) ($\equiv$ for none). Thus, the completion of the Boolean algebra BA-3, starting from (1 0 0) ($\equiv \forall$) and (0 0 1) ($\equiv \Phi$) (of QPL) via the following steps, gives automatically (0 1 0) ($\equiv \Sigma$), and there is no incompleteness in EQPL.

Let $\underline{a}$ = (1 0 0), $\underline{b}$ = (0 0 1). Then, their complements are $\langle a | M | = \langle c | = (0\ 1\ 1)$, and $\langle b | M | = \langle d | = (1\ 1\ 0)$. The Boolean product $\underline{c} \otimes \underline{d}$ gives $\langle c | V | d \rangle = (0\ 1\ 1) \otimes (1\ 1$ = (0 1 0).

On the other hand, we shall now show that this state (0 1 0), which occurs only in BA-3, is outside the domain of SNS also, (which is representable only by BA-2). In this

sense FC (represented by SNS) is itself incomplete. In fact, it can be shown to arise out of statements that can be made in SNS logic making use of reverse connectives (of Boolean operations) and it then has all the properties of $\sum$. The steps are as follows. If we examine the truth tables, Table of [1] and Table 3 of [2] , it will be seen that the following hold good:

$\langle c \mid V \mid a \rangle = \langle x \mid$, with $\underline{\underline{c}} = T$, $\underline{\underline{a}} = T$, gives $\underline{\underline{x}}' = T$ or D (30a)
i.e. 'D', but 'not F'

$\langle d \mid V \mid a \rangle = \langle x \mid$, with $\underline{\underline{d}} = T$, $\underline{\underline{a}} = F$, gives $x'' = F$ or D (30b)
i.e. 'D', but 'not T'

Now, $\underline{\underline{x}} = \underline{\underline{x}}' \underset{\sim}{V} \underline{\underline{x}}''$ gives "D, but "not T" and "not F". This is a state not describable in SNS, where D (= T or F) and 'not T' is F, so that "D and $\neg$T" with $\neg$F is a contradiction (X).

Thus, in SNS (EA-2) $\underline{\underline{x}}$ is a contradiction, if $\underline{\underline{x}} = \underline{\underline{x}}' \underset{\sim}{V} \underline{\underline{x}}''$ where $\underline{\underline{x}}'$ and $\underline{\underline{x}}''$ are as in (30a) and (30b). However, if we go

to BA-3, the following are possible:

$\underline{\underline{c}}$ = (1 0), $\mathcal{a}$ = (1 0 0), gives χ' = (1 0 0) or (1 1 0) or (1 1 1) (31a)

and

$\underline{\underline{d}}$ = (1 0), $\mathcal{b}$ = (0 0 1), gives χ'' = (0 0 1) or (0 1 1) or (1 1 1) (31b)

Hence $\chi' \otimes \chi''$ = (0 1 0) or (1 1 1) (31c)

We get (0 1 0) as one of the possibilities, viz "some" (Σ) and the other possibility is "universal doubt" (Δ) $\equiv$ may be for all, may be for some, may be for none. Leaving out Δ , which is the state of no information content for χ , we see that the state Σ , "for some", emerges clearly as a new possible state of doubt, with absence of certainty.

It is rather strange that all these shades of doubt were envisaged by Jaina Philosophers of 2000 year ago. (See [1], [2] , [3]), but the interesting point is that 2-valued logic (CL $\equiv$ BA-1) when properly completed by extending it to the four states of BA-2 in SNS, is still not complete. It leads on to BA-3.

(b) If SNS is complete then EQPL is also complete

The procedure adopted in showing that CL is complete is to show that any argument, which has, as inputs, only the states T or F, will lead to outputs of only T or F. The possibility of "T or F", as with $\underline{a} \Longrightarrow \underline{b}$ and $\underline{a} = F$, when "$\underline{b}$ can be T and can also be F," is included in the completion of the ~~argument~~ list of allowed states.

We can make the conditions for completion more compact in SNS, by allowing the four states T, F, D, X, homologous to (1 0), (0 1), (1 1), (0 0) of BA-2, to form the complete set of states for PC. Then any matrix relation, unary direct and reverse, and binary direct and reverse, gives back again only one of these four states as the output(s) of a sentence, or an argument. We can then say that PC(BA-2) is complete. (But, we have seen that it goes over into states of BA-3, if the symbolic connective $\underline{\vee}$ ($\otimes$) is reversed, but not in the direct form, as when $\otimes$ is used $\left[\underline{a} \underline{\vee} \underline{b} = \underline{c}\right)$.

In exactly the same way, the structure of matrix connectives in EQPL (see [2] for details) again leads only to an EPL (BA-3) state, when the canonical form of the input states is only of the 8 possible ones in EQPL. This is so for all unary direct and reverse, and binary direct and reverse connectives of the matrix type. It is also true for the symmetrical connectives $\oplus$ and $\otimes$ in the 'direct' form of application. Hence, EQPL (BA-3) is as complete as the SNS form of PC (BA-2). Every output is one of the eight Boolean 3-vectors, and leads to closure and completeness of EQPL.

We say, in effect, that Gödel's incompleteness theorem, for QPL, (see [4], p. and [8],) is not there. This is best seen by the following statement of this theorem:

Gödel's incompleteness theorem

"In any theory based on first order predicate calculus containing quantifiers, there are theorems which are true, but which cannot be proved to be always true, or always false" ("always" may be replaced by "completely") (32)

In effect, if $\underset{\sim}{s}(x)$ is the statement (theorem) under consideration, the theorem says that $\underset{\sim}{s}(x)$ is T for some x, but cannot be proved to be true for all x, or not true for all $\underset{\sim}{x}$ (i.e. true for no $\underset{\sim}{x}$). In our vector-matrix formalism for QPL, this means that $\underset{\sim}{s}(x)$ is true only for $(\leq x)$, and not for $(\forall x)$, and also not for $(\underset{\sim}{\Phi}\, x)$.

Since the quantifier state $(\leq x)$ is a well-acceptable one for EQPL, if this possibility is included into the complex of axioms for EQPL, then there is no "incompleteness" produced by some "theorems" or statements in QPL, having the state $\leq$. Therefore, to the extent to which SNS is complete, EQPL is also complete. (But, on reversing statements containing the connective $\underset{\sim}{\vee}$, we can get states outside EQPL and belonging to BA-m ($m = 2^7 - 1$), and to this extent, EQPL, based on BA-3, is incomplete; but so are all multi-valued logics based on any BA-m ($m \geq 2$) incomplete.

5. Consistency and Completeness of all Multi-valued Logics

(a) Theory for n-valued logic:

— As described in Ref [2], n-valued logic becomes naturally representable by n-element Boolean vectors and (n x n)-valued Boolean matrices as connectives. Under these conditions, it is extremely easy to show that all unary and binary relations, whether of the direct type or of the reverse type, gives rise only to an n-element Boolean vector, or a 2-element Boolean vector, for the truth value of the relation concerned. Hence the algebra of n-element Boolean vectors, containing 2^n possible vectors, is closed with reference to all $|n \times n|$ matrix operations as mentioned above. This is a standard concept of completeness of a theoretical structure.

On the other hand, the Boolean operations ⊕ and ⊗ also take over all n-element Boolean vectors connected by them into another n-element Boolean vector in the set. Consequently, these two operations in the forward direction also <u>do not give</u>

any element outside the algebra composed of n# basic vectors, # having the element unity at each of the n# positions of the n-element vector.

However, as mentioned earlier and also in Ref [2] , the set of vectors in BA-n is not closed with reference to reversal of the operations ⊕ and ⊗. In this case, all possible vectors (produced by such reversals and combinations of ~~vectors~~ them, obtained by applying all relevant operators of BA-n), ~~produced of the reversal by Boolean connectives~~ when put together, give rise to a Boolean algebra BA-n' where $n' = 2^n - 1$.

The above statements are completely valid for all multi-valued logics and it is seen that no multi-valued logic isomorphous with BA-n is closed with respect to all operations (both matrix and non-matrix) acting on the vectors. They are, however, closed with respect to conventional logical operations which depend only on matrix operation and the forward application of

⊕ and ⊗. Thus, there is complete consistency for a single BA-n in its logical application and also a "closed" character, which can be given the name "completeness", as it is normally understood. However, strictly no finite Boolean algebra is closed (under reversal of ⊕ and ⊗), and therefore no n-valued logic can escape the requirements of a higher valued logic if all its consequences are to be examined.

(b) Particular Comments for SNS and EQPL:

As already stated, propositional calculus becomes rich and fully valuable only when it is extended to SNS logic and the new concept that is mainly introduced in SNS is the inclusion of the two new states $D = T \oplus F$ and $X = T \otimes F$ to the two states T and F already understood in propositional calculus. From the point of view of acquisition of knowledge in the field of semantics, as distinct from logic, the state D being transformed into the state T or F is the supreme objective of

any scientist (theorist) of any branch of knowledge. In terms of SNS logic, this is done by means of the vidya (= Knowledge (Sanskrit)) operator ($\underset{\sim}{V}$) applied between information first available in the form of a vector $\underset{=}{a}_1$ in the state D, and fresh knowledge coming about the same object in the form of a definite-state logical vector $\underset{=}{a}_2$ (T say). Then the resultant of the two types of information $\underset{=}{a}_1$ and $\underset{=}{a}_2$ is to give rise to

$$\underset{=}{a}_1 \underset{\sim}{V} \underset{=}{a}_2 = D \underset{\sim}{V} T = T \qquad (33)$$

This concept, that doubt is always there about anything, is the fundamental basis of the so-called Syād-vāda of the ancient Jaina philosophers of India. They considered that one can only say about anything — "may be it is true, may be it is false". This is because no theory can be complete, and, at no time, can one assert that "This is the last word about this thing". Some new knowledge or factor may turn up which has not been previously, which

may alter the statement from "yes" to "no". Thus, ancient Indian epistemology relies heavily on the concept of doubt superposed on definiteness leading to definite knowledge. (The definiteness may be either T or F).

Similarly, the same Jaina philosophers somehow got hold of the concept that even doubt can be of several different types and they had a word for the type of doubt which can, at the same time, be neither true nor false, which, in our notation is expressed by the EQPL state $\sum \equiv (0\ \ 1\ \ 0)$. The name given for this was "avaktavya" which, strictly translated means unstatable, or indescribable. This term is quite understandable because, in the normal way, when there is doubt, we have the situation that we cannot decide between truth and falsehood; but apparently, they realized that, in arguments there come situations where something is not always true, nor is it always false, but that it is still possible to talk of that entity which is "sometimes true" — avaktavya. They even listed the 7 possible states of EQPL, including the three basic states, true, false and avaktavya (see [1] , [3]).

Perhaps a very simple illsutration may indicate that this state is of extremely common occurrence. Consider an integer N and ask whether the proposition "N is a prime" is always true or always false. It is neither; but "N is a prime" is valid sometimes. Consider elementary propositions in number theory. Thus, "N is rational" is true for ($\forall$ N). "N is an irrational number" is true for (Φ N), while "N is a prime" is true only for (Σ N). In fact it is the state that is obtained by saying "there exist primes"($\exists$ N) and "not all are primes" ($\neg(\forall$ N)). Thus, the state (Σ N) is obtainable very simply by using the two common quantifiers "there exists" ($\exists$) and "not for all" (Λ), and forming $\exists \otimes \Lambda$.

In view of what has been said above, one does not have to worry at all that some propositions in mathematics cannot be proved to be either always true or always false. It is

is perfectly common and readily occurring. To say more than this — such as to determine the conditions under which an object or statement is D (as our theorem about ω being both equal and not equal to itself) or Σ (as with primes among integers)—would take us outside mathematical logic into the realm of philosophy of Knowledge.

Acknowledgement

The author wishes to thank Mr. M. Suresh for assistance in the preparation of this paper through several drafts. The work was supported by a special grant from Council of Sciehtific and Industrial Research.

References

1. Ramachandran, G.N. Current Sci. Vol 51, No.13, p.625-636(1982)

2. Ramachandran, G.N. Current Sci. (1983), in press, to appear in April issues.

3. Hiriyanna, M. "Outlines of Indian Philosophy", George, Allen and Unwin, London (1932), p. 150.

4. Stoll, R.R. "Set Theory and Logic", W.H. Freeman & Co., San Francisco, 1963.

5. Russell, B. "Introduction to Mathematical Philosophy", Simon and Schuster, New York, 1982.

6. Kennedy, J.G. "Encycl. Britannica", William Benton, Chicago, 1965, Vol. 20, p. 313D.

7. Black, Max "Encycl. Britannica", William Benton, Chicago, 1965, Vol 2, p. 53.

8. Suppes, P. "Introduction to Logic", Van-Nostrand, New York, 1968

A NEW TECHNIQUE OF CRYSTAL STRUCTURE ANALYSIS

(Report prepared for a discussion of this technique on July 18 to 21, and a brief outline of the further studies made upto August 12.)

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(For private circulation only)

MATPHIL Reports No.31, August 1983

PREFACE

This is a report of the initial stages of the studies made on a novel procedure to obtain a low-resolution electron density map of a crystal structure, with broadened peaks. It uses a large temperature factor and a sub-lattice grid of atoms at fixed locations (x_i,y_i), whose "weights" (m_i) are the only quantities that are varied. To start with, hypothetical structures with gaussian atoms in a 2D unit cell, with the lowest plane group symmetry p1, have been examined. The R-value always drops down in the refinement procedure, from high values of 0.6 to 1.0, down to 0.2 with 4X4 grids to 8X8 grids in the unit cell.

The procedure is such that if R is made lower, there should be a reduction in the integral of the magnitude of the difference in e.d. between the real structure and the approximated structure. This can be tested via minimum function procedures, which has yet to be done.

A number of examples have been tested, and some of these are summarized in Tables 1 to 7. However, this report is only a working paper so that it may form a basis for the discussions which are taking place from July 18 to 21. It is not for general circulation.

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When this report was written in detail, an error was noticed in our programs, in that the factor T(H) in Eqn. 12(b) was omitted in the set of formulae used for calculating the data presented in Sections 1 to 4. However, this has the effect of only a weighting factor in the formulae and the end results described herein are not seriously affected. The correct formula is being tested and appears to work even better than the data presented here. They are described in Section 5.

The programming and calculations mentioned in Section 4 were carried out by T.A. Thanaraj, CCMB, Hyderabad, while those in Table 6 and related ones were done by Thanaraj along with S.S. Rajan. The application to real atoms, shown in Table 7 were programmed and calculated by K.I. Varughese, on leave from NRC, Canada, working in Bangalore from July 18 to August 12.

C O N T E N T S

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Ab-initio Grid-approximation Method of Determining Crystal Structures using only Structure Amplitudes

1. Introduction:

In standard crystallographic practice, the initial determination of atomic locations is made by a method of trial and error, and only afterwords are exact calculations made for refining the preliminary structure. The so-called "direct methods" are highly useful in this initial stage, but they also require the intermediary of the crystallographer to determine which of the possible solutions that are turned out by the computer are suitable for further manipulations. It is the experience of crystallographers that, if the R-value is less than about 0.30, then standard least-squares techniques car. be employed for reducing it to as low a value aspossible, depending on the accuracy of experiental data.

It is well known that the direct methods are more difficult for non-centrosymmetric structures than for centrosymmetric ones, and they are most difficult for crystal structures having the space group symmetry P1.

We have been working on a technique which can be used for the initial steps of structure analysis and which gives low R-values of the order of 0.20, using only the observed intensities and structure amplitudes, without feeding in any phase information. The principle of this method is to approximate the electron density of the actual crystal structure by a set

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We have been working on a technique which can be used for the initial steps of structure analysis and which gives low R-values of the order of 0.20, using only the observed intensities and structure amplitudes, without feeding in any phase information. The principle of this method is to approximate the electron density of the actual crystal structure by a set

of broadened atoms located at suitable grid points in the unit cell. The locations, governed by the grid intervals between atoms are chosen for a particular choice of the breadth of the atomic electron distribution so that the grid atoms overlap suitably. The "strength" (or total electron count) of the atom at each grid point is the only quantity that is varied. This is equivalent to solving the crystal structure at a low resolution. Having obtained the best structure for a particular resolution, the breadth of atoms (as determined by the temperature factor B) is reduced and the grid points are also brought closer together. Then the strengths of these new grid atoms are first determined by interpolation from the old ones, and then a suitable mathematical technique of refinement based on the least-squares approach, is applied to these to get a better-resolved approximation to the real structure.

The technique has been tested so far only for two-dimensional structures in the plane group p1, Even if the initially chosen strengths (m-values) give an R-value as large as .7 or even 1.0, the R-value rapidly comes down, in some 6 to 10 cycles of the refinement process to 0.25, or even less. We have not checked the nature, or accuracy, of the structure thus determined with reference to the actual crystal structure which it represents, and this is one of the things that must be done as early as possible.

In the first part of the paper (Sections 2 to 4), the relevant formulae are given for a hypothetical case of gaussian atoms

in a two-dimensional crystal structure, and the main results obtained are illustrated by tabular data. In sections 5 onwards, the relevant formulae for real atoms having atomic structure factors varying with $(\sin\theta)/\lambda$ (according to well-known formulae) are worked out, and the related formulae for a 3-D structure are written out (for a triclinic crystal with P1 symmetry, but for a cubiccell). These have to be implemented on the computer and the technique tested for its capabilities. This is done in Part II.

2. Theory for 2D structures with gaussian atoms.

For simplicity in explaining the theory, we assume that the structure has symmetry p1, but that the unit cell is a square with each side of length unity. The atomic positions are given by (x_{j1},x_{j2}), and their scattering factors are $f_j \exp(-B(h_1^2+h_2^2)/4)$, for j = 1 to J. We assume, again for simplicity, that all the atoms in the structure have the same scattering factors f_j equal to unity (although f_j's can be taken to have any values, if necessary). Thus, in this equal atom case, we take $f_j = 1$ for all j. With these conditions, we have the well-known formula (1) for the structure amplitude $F(h_1,h_2)$:

$$F(h_1,h_2) = \sum_{j=1}^{J} f_j \exp\left[-B(h_1^2+h_2^2)/4\right] \exp 2\pi i(h_1x_{j1}+h_2x_{j2}) \qquad (1)$$

(a) Grid approximation:

The atoms in the unit cell are approximated by gaussian atoms i (i = 1 to I) having strengths m_i, by having the same B-values as the actual structure (for reasons that will be clear

in Section 4), located at grid points separated by intervals $1/I_1$, both along the x_1- and $1/I_2$ along the x_2-direction. For simplicity, we take $I_1=I_2$. Hence, i ranges from 1 to I_1^2 (= I). The unit cell is divided into I_1^2 square subcells, as in Fig.1, and the trial grid atoms may be located either at the corners of the cells, or in their centres, as in Fig. 1(a) and 1(b).

Fig.1. Location of atoms of strength m_i at (a) $x_1 = (i_1-1)/I_1$, $x_2 = (i_2-1)/I_1$, and (b) $x_1 = (i_1-\frac{1}{2})/I_1$, $x_2 = (i_2-\frac{1}{2})/I_1$ (i_1,i_2 = 1 to I_1). The value $I_1=4$ is taken for illustration, and the numbers against the atoms are the i-values.

It is readily seen that the structure amplitude $G(h_1,h_2)$ of the approximating structure in Fig.1(a) is given by:

$$G(h_1,h_2) = \sum_{i=1}^{I} m_i g_i \exp[-B(h_1^2+h_2^2)/4] \exp 2\pi i(h_1(i_1-1)+h_2(i_2-1))/I_1 \qquad (2a)$$

and

$$G(h_1,h_2) = \sum_{i=1}^{I} m_i g_i \exp[-B(h_1^2+h_2^2)/4] \exp 2\pi i(h_1(i_1-\tfrac{1}{2})+h_2(i_2-\tfrac{1}{2}))/I_1 \qquad (2b)$$

As in the case of f_j's, g_i are all taken to be unity for simplicity, so that we need determine only the strengths of atoms m_i, namely as in Eqns. (3a) and (3b), corresponding to Figs. 1(a) and 1(b) respectively:

$$m_i = m_{i_1,i_2} \quad \text{at } x_{1i} = (i_1-1)/I_1,\ x_{2i} = (i_2-1)/I_1 \qquad (3a)$$

$$m_i = m_{i_1,i_2} \quad \text{at } x_{1i} = (i_1-\tfrac{1}{2})/I_1,\ x_{2i} = (i_2-\tfrac{1}{2})/I_1 \qquad (3b)$$

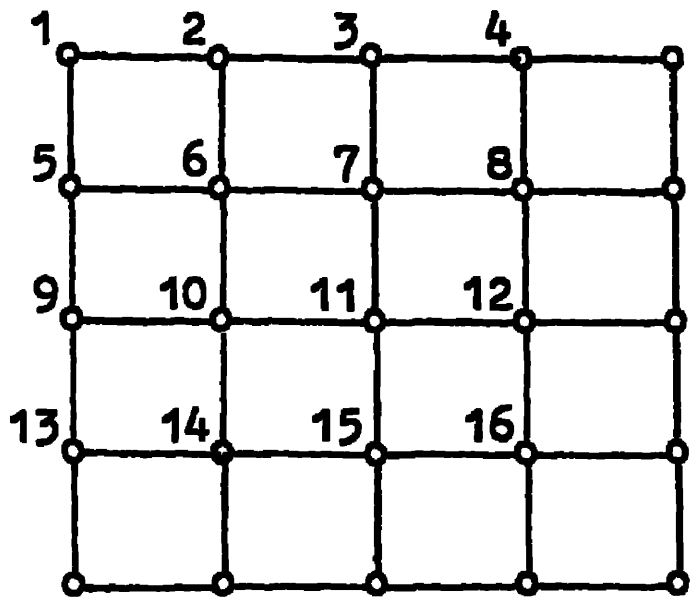

Fig.1(a): I_1=4, i=1 to 16, corresponding to Eq. (3a).

1_o	2_o	3_o	4_o
5_o	6_o	7_o	8_o
9_o	10_o	11_o	12_o
13_o	14_o	15_o	16_o

Fig.1(b): I_1=4, i=1 to 16, corresponding to Eq. (3b).

It is readily verified that i is related to i_1 and i_2 by Eq. (3c)

$$i = (i_2-1)I_1 + i_1 \qquad (3c)$$

(b) Principle of the refinement procedure:

We know that the electron density everywhere is positive in a crystal structure and we implement this condition in the idealised case considered here, by taking all the atoms to be representable by gaussian electron density distributions given by

$$\rho_j (x_1,x_2) = p_j \exp [-K \{(x_1-x_{j1})^2 + (x_2-x_{j2})^2\}] \qquad (4)$$

If the grid points are taken such that the approximating atoms have sufficient enough overlap, we can expect that the approximating atoms can reasonably represent the electron density distribution of the crystal structure. In other words, the function

$$\rho(x_1,x_2) = \sum_{j=1}^{J} \rho_j (x_1,x_2) = \sum_{j=1}^{J} p_j \exp [-K\{(x_1-x_{j1})^2+(x_2-x_{j2})^2\}] \qquad (5)$$

is taken to be approximated by the function,

$$\rho'(x_1,x_2) = \sum_{i=1}^{I} m_i \exp [-K'\{(x_1-x_{1i})^2+(x_2-x_{2i})^2\}] \qquad (6)$$

(K' is made equal to K for the reason stated above). This is a good conjucture for the real space crystal structure (which, in our case, is a unit cell of spacing unity and of two dimensions), and if K and L are suitably chosen, m_i should be determinable theoretically.

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We take the equivalent of this conjucture in the Fourier transform space, by making the best fit of $|F(h_1,h_2)|$ and $|G(h_1,h_2)|$. This is done by minimising the well known crystallographic parameter R (namely the reliability index) given by,

$$R = \sum_H ||F(H)| - |G(H)|| \; / \; \sum_H |F(H)| \qquad (7)$$

using the least-squares procedure, varying only m_i (for i=1 to I) for this purpose.

The relevant formulae are given in Section 3, and Section 4 gives an outline of the results obtained usimg them, for symmetry p1, and using the grid atom positions as in Fig.1(a). Since R is not an analytic function of x_{1i}, x_{2i} and m_i, we use the assumption that R will decrease if all $\Delta|F(H)|$ given by Eq. (8)

$$\Delta|F(H)| = (|F(H)| - |G(H)|) \qquad (8)$$

are minimised in the least-squares sense - i.e., we seek to find the values of m_i (given x_{1i}, x_{2i}) for which $\sum_H \Delta|F(H)|$ is a minimum, which is ideally achieved if each term $\Delta|F(H)|$ is sought to be made zero.

3. Least squares formulae for reducing the R-value.

(a) General

In the expression (7) for the R-value, $|F(H)|$ ($= |F(h_1,h_2)|$) are assumed to be given. Most of the tests described in the next section have been performed using the theoretical values of $|F(H)|$, with no experimental errors, althogh the effects of artificially

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introduced errors of mean value 5 to 15% have been tested, which are described at the end of Section 4. The quantities G(H), on the other hand, are theoretical expressions, given by Eq. 2(a), with $g_i = 1$ for all i. Hence, we obtain the following formulae in (9) and (10).

We denote the common temperature factor of all grid atoms $H = h_1$, by T(H). Thus,

$$\exp\left[-B(h_1^2+h_2^2)/4\right] = T(h_1,h_2) = T(H) \qquad (9a)$$

Then, the real and imaginary parts $G_c(H)$, $G_s(H)$, of G(H) are

$$G_c(H) = \sum_{i=1}^{I} m_i\, T(H) \cos\theta(H,i) \qquad (9b)$$

$$G_s(H) = \sum_{i=1}^{I} m_i\, T(H) \sin\theta(H,i) \qquad (9c)$$

where T(H) is given by (9a), and

$$\theta(H,i) = 2\pi(h_1x_{i1}+h_2x_{i2}) \qquad (9d)$$

with x_{i1}, x_{i2} given by (3a), or (3b), as the case may be. Then, if we write

$$G(H) = |G(H)| \exp i\,\alpha_H \qquad (10a)$$

then

$$|G(H)| = \left\{G_c^2(H) + G_s^2(H)\right\}^{\frac{1}{2}} \qquad (10b)$$

and

$$\tan\alpha(H) = G_s(H)/G_c(H) \qquad (10c)$$

Considering Eq. (8), since F(H) are constants, we obtain

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$$\frac{\partial \Delta|F(H)|}{\partial m_i} = \frac{\partial |G(H)|}{\partial m_i} \quad \frac{1}{|G(H)|}\frac{\partial}{\partial m_i}\left(G_c^2(H)+G_s^2(H)\right) \qquad (11a)$$

$$= \frac{1}{2|G(H)|}\left[2G_c(H)\frac{\partial G_c(H)}{\partial m_i} + 2G_s(H)\frac{\partial G_s(H)}{\partial m_i}\right] \qquad (11b)$$

We denote

$$\frac{G_c(H)}{|G(H)|} = C_c(H) \quad ; \quad \frac{G_s(H)}{|G(H)|} \quad C_s(H) \qquad (11c)$$

and we have, from (9b) and (9c),

$$\frac{\partial G_c(H)}{\partial m_i} = T(H)\cos\theta(H,i) \quad ; \quad \frac{\partial G_s(H)}{\partial m_i} = T(H)\sin\theta(H,i) \qquad (11d)$$

Thus, the analytic expression for $-\partial\Delta|F(H)|/\partial m_i$ in terms of $\frac{\partial|G(H)|}{\partial m_i}$ is

$$\frac{\partial \Delta|F(H)|}{\partial m_i} \quad \frac{\partial|G(H)|}{\partial m_i} = p(H,i) \qquad (12a)$$

$$= T(H)\left[C_c(H)\cos\theta(H,i) + C_s(H)\sin\theta(H,i)\right] \qquad (12b)$$

Thus, we wish to solve the set of equations (13a) below for Δm_i,

$$\sum -\frac{\partial\Delta|F(H)|}{\partial m_i}\delta m_i = \Delta|F(H)| \qquad (13a)$$

where the l.h.s. is a linear sum of δm_i multiplied by $p(H,i)$, while the r.h.s. is a number obtained from the data m_i that are fed in, which gives $|G(H)|$. Denoting δm_i by $\delta(i)$ and $\Delta|F(H)|$ by $\Delta(H)$, we get the following set of linear equations to be solved

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$$\sum_{i=1}^{I} p(H,i)\,\delta(i) = A(H), \quad H = 1 \text{ to } H_{max} \qquad (13b)$$

If the number of reflections H (= (h_1,h_2)) (namely H_{max}) is larger than I (the number of grid atoms), then we can solve these equations by producing I normal equations in I unknowns ($\delta(1)$) by multiplying each equation by the coefficient p(H,1) (for $\delta(1)$) and summing them. Thus, denoting

$$\sum_{H=1}^{H_{max}} p(H,1)\,p(H,i) = q(1,i) \qquad (14a)$$

and

$$\sum_{H=1}^{H_{max}} p(H,1)\,A(H) = \Delta(1) \qquad (14b)$$

The normal equations to be solved are

$$\sum_{i=1}^{I} q(1,i)\,\delta(i) = \Delta(1) \quad (1 = 1 \text{ to } I) \qquad (15a)$$

In principle, these I equations in I unknowns can be solved by matrix inversion . If we denote the inverse of q(1,i) by $q^{-1}(i,1)$, then

$$\delta(i) = \sum_{1=1}^{I} q^{-1}(i,1)\,\Delta(1) \qquad (15b)$$

In practive, we have found that the "diagonal approximation" is good enough, and we can obtain $\delta(i)$ from the equations

$$\delta(i) = \Delta(i)/q(i,i) \qquad (15c)$$

The m_i-values then take new values m_i', given by

$$m_i' = m_i + \delta(i) \qquad (16)$$

(b) Iteration Procedure for a choice of the grid sub-division.

As mentioned earlier, our procedure is to refine m_i so that a closer and closer approximation of the electron density (e.d.) of the crystal structure is obtained. Thus, having obtained the set m_i' (i= 1 to I), we should check if any m_i' are negative. If so, such m_i' are put equal to zero, since the e.d. cannot be negative anywhere.

Further, the new set m_i' is "normalized" - i.e. $\sum_{i=1}^{I} m_i'$ is made equal to $\sum_{j=1}^{J} f_j$. For this, let

$$\sum_{j=1}^{J} f_j = M \qquad (17a)$$

where M stands for the total electron count in the unit cell, and let

$$\sum_{i=1} m_i' = M' \quad , \quad \text{and } S = M/M' \qquad (17b)$$

Then, S is the normalizing factor by which each m_i' is multiplied to give the m_i's to be used for the next iteration. Thus,

$$m_i(2) = Sm_i' \quad ; \quad m_i(n+1) = Sm_i'(n), \text{ in general} \qquad (18a)$$

where n is the number of the iteration, performed using Eqns. (9) to (16). In fact, even for the first iteration (n=1), the inputs are labelled m_i', and the m_i's put in Eqns. (9b) and (9c) are

$$m_i(1) = Sm_i' \qquad (18b)$$

For each iteration, R is calculated, and the procedure described in Section 3(a) will reduce R, provided B is chosen

suitably for each I_1, I_2. If $I_1=I_2$ as we have tested so far for a square unit cell, the following simple formula for B and K has been empirically found to give the best refinement:

$$K = (2.5 \text{ to } 3.5)\ I_1 \quad ; \quad B = (5 \text{ to } 3.5)/I_1 \qquad (19a)$$

Two values of B (or K) are chosen, and the one that gives the better refinement of R is taken for further processing. As will be seen from Section 4, some 10 iterations reduce R from about 0.6 to 0.8 to about 0.2. Generally, the refinement is stopped when the reduction $|\Delta R|$ in R for an iteration is less than 0.01 (or 0.005, if needed).

In fact, B and K are related by the equation

$$4\pi/K = B \qquad (19b)$$

Hence, the formulae (19a) for B and K lead to gaussian atoms having a half-width of the same order as the spacing $1/I_1$ ($=1/I_2$ of the subcell used for the grid-approximation structure.

(c) Successive choices of finer grids.

Generally, $I_1=I_2=4$ is found to be a good choice for the first grid sub-division to be chosen. In this case, $I=I_1I_2=16$, and sixteen m_i's have to be refined. Section 4(a) gives a typical example of the way the refinement proceeds. After the refinement is completed for this grid, the m_i's for $I_1=I_2=4$ may be interpolated to give the starting m_i's for the next larger I_1 e.g. $I_1=I_2=5$ or 6. (The interpolation procedure is given in Section 4(b)). Then, these m_i's for the 6X6 grid are refined

in exactly the same manner, but using a new value of B for I_1=6, as given by (19a).

In doing this, the value of $|H_1| = |H_2|$, the maximum values of h_1 and h_2, have to be chosen, such that H_{max} is 2 to 4 times the magnitude of I. The way this is done is described in Section 4(α). Usually, on interpolation from a 4X4 to a 5X5 cell, R goes up from about 0.20 to about 0.50 and on iterating, comes down to 0.25 or less.

4. Practical Details of the Computations.

(a) Refinement of R-values.

It has been verified that an iterative procedure, using (for each cycle of iteration) Eqns. (2) to (18), has the property of continuously reducing the value of the "residual" (R), irrespective of whatever be the initial m_i-values that are fed in. For example, this was tested for the structure denoted by the symbol FSG2-1, with ten equal atoms in the unit cell at cocrdinates (x_{j1},x_{j2} ; j = 1 to 10), as in Table 1(a). This structure

Table 1: Typical examples of the first stage of refinement of a 2D structure (ncs) approximated by a 4X4 grid.

is non-centrosymmetric and belongs to the plane group p1, although the unit cell is a square. This was sought to be approximated, starting from an arbitrarily chosen 4X4 grid structure (GSG2-1),

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Table 1: Typical examples of the first stage of refinement of a 2D structure (ncs) approximated by a 4X4 grid.

(a): Structure to be solved FSG2-1 (F-structure, General, 2D, Example 1).

	x_{j1}	x_{j2}			x_{j1}	x_{j2}	f_j
1	0.00	0.30	1.0	6	0.95	0.70	1.0
2	0.35	0.20	1.0	7	0.60	0.90	1.0
3	0.40	0.45	1.0	8	0.35	0.80	1.0
4	0.60	0.30	1.0	9	0.30	0.60	1.0
5	0.90	0.45	1.0	10	0.15	0.80	1.0

(b): Initial and Final 4X4 Grid Structures using GSG2-1 as the starting point (K=10, $H_1=H_2=4$, $H_{max}=41$)*+

Initial GSG2-1 grid				Final 4X4 grid after 11			
1.25	1.25	1.25	1.25	1.77	0.07	0.69	1.37
1.25	1.25	1.25	1.25	1.28	0.07	0.97	0.33
0.00	0.00	0.00	0.00	0.74	0.56	0.19	0.74
0.00	0.00	0.00	0.00	0.16	0.22	0.84	0.00
R(initial) = 1.235				R(final) = 0.193			

* x_{i1}, y_{i1} for i = 1 to 16 according to Fig.1(a)

\+ m_i-values normalized to make $\sum_i m_i = \sum_j f_j = 10.00$

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with m_i-values as shown in Table 1(b). In this structure, one half of the cell consists of 8 equal atoms and no atoms at all are present in the other half of the cell. In order to make $\sum_{j=1}^{10} f_j = \sum_{i=1}^{16} m_i$, each of the equal atoms in the initial structure GSG2-1 is given a weight 1.25 (It is to be noted that the initial grid structure GSG2-1 has a centre of symmetry and belongs to the plane group $p\bar{1}$. As will be seen below, this makes no difference to the procedure of getting a final non-centrosymmetric structure, since the output from the first cycle of the iteration itself is non-centric.)

As a result of various trials, the empirical value of the best K for this problem was taken to be K = 10 (of Eq.(19)). Similarly, in the reciprocal space, the maximum values of h_1, h_2 (namely, H_1, H_2) were both made equal to 4 and only one independent half of the $|F|$-values in the reciprocal space (h_1,h_2: was used (as usual) including, however, (h_1,h_2) = (0 0). This yields 9X5 - 4 = 41 structure amplitudes $F(h_1,h_2)$ for the refinement of 16 m_i-values. The results of refinement will be presented during the practical discussions, showing that m_i's continuously change to give successively smaller and smaller R-values, starting initially with R = 1.235. After 11 cycles of refinement, R comes down to 0.193, and the 16 final m_i-values are also shown in Table 1(b). The data in Tables 1(a) and (b) are from output No. 81, which contains also results for still smaller grid subdivisions with I_1=5 and 6 which were tried. These latter are briefly listed in Table 2. The interpolation procedure is des-

Table 2: Initial and final m_i-grids and R-values for the interpolated 5X5 and 6X6 cases of GSG2-1 of Table 1(b)**

(a): 5X5 grid: I_1=5, K=15, H_1=H_2=5, H_{max}=61.

R(initial) = 0.514

1.07	0.20	0.28	0.59	0.88
0.84	0.22	0.35	0.47	0.45
0.53	0.30	0.27	0.33	0.40
0.31	0.27	0.27	0.27	0.27
0.30	0.16	0.34	0.36	0.19

R(final) = 0.288

1.35	0.19	0.20	0.61	1.16
1.06	0.00	0.47	0.64	0.00
0.58	0.39	0.33	0.04	0.56
0.20	0.26	0.33	0.34	0.42
0.19	0.02	0.27	0.39	0.00

(b): 6X6 grid: I_1=6, K=15, H_1=H_2=6, H_{max}=85.

R(initial) = 0.468

0.90	0.25	0.12	0.28	0.53	0.27
0.72	0.14	0.19	0.34	0.31	0.22
0.52	0.23	0.22	0.21	0.19	0.27
0.29	0.23	0.21	0.18	0.20	0.30
0.14	0.13	0.18	0.23	0.22	0.17
0.26	0.07	0.14	0.24	0.23	0.15

R(final) = 0.289

1.06	0.25	0.10	0.27	0.60	1
0.89	0.00	0.08	0.43	0.32	0
0.63	0.25	0.29	0.32	0.06	0
0.25	0.25	0.15	0.14	0.11	0
0.11	0.16	0.18	0.40	0.27	0
0.25	0.01	0.06	0.25	0.05	0

* All grid structures are as in Fig.1(a).

\+ m_i-values normalized to correspond to the F-structure in Table 1(a) ($\sum_i m_i = 10.00$).

cribed in the next section 4(b).

Table 2: Initial and final m_1-grids and R-values for the interpolated 5X5 and 6X6 cases of GSG2-1 of Table 1(b).

The results obtained, using another centrosymmetric initial G-structure (GSG2-5), for I_1 = 4,5,6,8, and varying K and H_1=H_2, are summarized in Table 3. It will be seen that the exact values of the latter two parameters do not affect the finally refined G-structure very much, for a chosen grid approximation.

By using a non-centric initial G-structure (GSG2-7), the starting R-value for the 4X4 grid is reduced to 0.561, as shown in Table 4, but its behaviour is still very similar to that in Table 3 thereafter. The R(final)'s are slightly lower than with GSG-2.

Table 3: Another example (Output No.82) of refinement from L=4 to L=8. (FSG2-1 and GSG2-5(c.s.)) .

Table 4: One more example (Output No.83 with the non-centric GSG2-7 input) for L=4 to L=6.

We shall now describe some practical details like interpolation, which has been implemented, and the calculation of the minimum function, which has been tried in a rough way, but has to be applied in a better manner.

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Table 3: Another example (Output No.82) of refinement from L=4 to L=8. (FSG2-1 and GSG2-5(c.s.))*

Grid	K	$H_1=H_2$	H_{max}	R(initial)	R(final)	No.of cycles
4X4	10	4	41	0.871	0.203	20
5X5	12.5	4	41	0.519	0.198	11
"	12.5	5	61	0.211	0.206	2
"	10.0	5	61	0.211	0.207	3
6X6	15.0	5	61	0.470	0.255	11
"	15.0	6	85	0.260	0.255	2
"	12.5	6	85	0.229	0.226	2
8X8	20.0	6	85	0.500	0.277	14
(Had to be stopped for lack of computer time)						

* GSG2-5 is (not normalized)

2	2	2	2
2	2	2	2
1	1	1	1
1	1	1	1

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Table 4: One more example (Output No.83 with the non-centric GSG2-7 input) for L=4 to L=6.*+

Grid	K	$H_1=H_2$	H_{max}	R(initial)	R(final)	No. of cycles
4X4	10	4	41	0.561	0.193	9
5X5	12.5	4	41	0.548	0.217	13
"	12.5	5	61	0.224	0.221	2
"	10.0	5	61	0.186	0.183	2
6X6	15.0	5	61	0.487	0.210	15
"	15.0	6	85	0.215	0.212	2

* This shows features quite similar to Tables 2 and 3.

+ GSG2-7 is (not normalized)

0	1	0	1
1	0	0	1
0	1	1	0
1	0	0	1

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(b) Grid Interpolation formula.

For the interpolation from the final output of m_i's for a $I_1 \times I_2$ grid (the I-grid) to determine the m'_i for i'=1 to I'(=$I'_1 I'_2$) for a $I'_1 \times I'_2$ grid (the I'-grid), a simple formulation was employed as shown below, for distributing each m_i at (i_1,i_2) to four grid points of the I'-grid. For convenience, we assume that the atomic coordinates of a grid are given by the simple formula

$$x_{11}=i_1/I_1,\ x_{12}=i_2/I_2,\ m_i=m(i_1,i_2),\ i=1 \text{ to } I_1 I_2 \qquad (20)$$

and we shall take the two cases of Eqns. (3a) and (3b) as modifications of the structure in (20) afterwards.

First, each (i_1,i_2) is convdrted into fractional numbers (may be integers) in the I'-grid. Let

$$I'_1/I_1 = c_1 \ ; \ I'_2/I_2 = \qquad (21a)$$

and let

$$c_1 i_1 = i'_1+i_{f1} \ ; \ c_2 i_2 = i'_2+i_{f2} \qquad (21b)$$

where i'_1, i'_2 are integers and i_{f1}, i_{f2} are fractions less than unity (may be equal to zero). Then, the contribution from $m_i(i_1,i$ to the strengths m'_i are the four I'-grid points (in 2D) enclosing it are given by (22a-d) - see Fig.2.

For (i'_1,i'_2)	$(1-i_{f1})(1-i_{f2})m_i$	(22a)
For (i'_1+1,i'_2)	$i_{f1}(1-i_{f2})$	(22b)
For (i'_1,i'_2+1)	$(1-i_{f1})i_{f2}m_i$	(22c)
For (i'_1+1,i'_2+1)	$i_{f1}i_{f2}m_i$	(22d)

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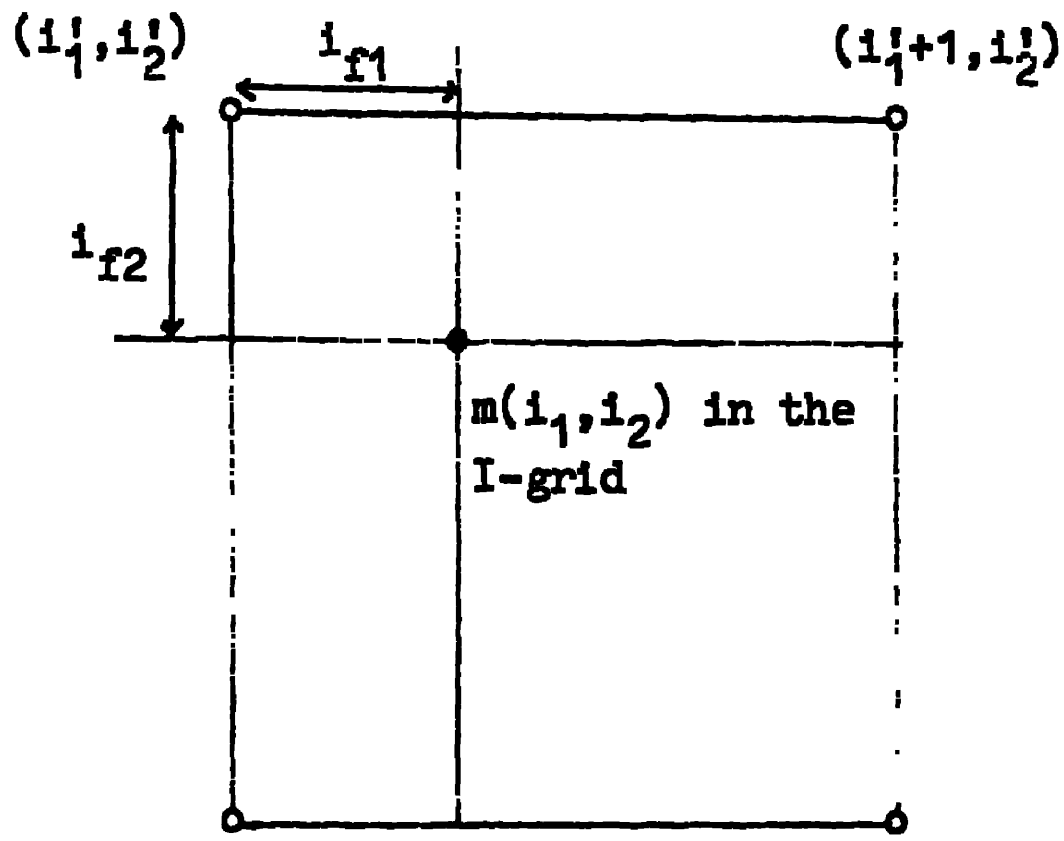

Fig.2. Symbols used in the interpolation procedure from the I-grid to the I'-grid.

It will be noticed that, if the m_i's are normalised, the interpolated $m_{i'}$'s are also normalized, and that the procedure described above is readily generalized to three dimensions.

Fig.2. Symbols used in the interpolation procedure from the I-grid to the I'-grid.

We shall now consider how Eqns. (21) and (22) are modified when the coordinates of the grid atom i, denoted by the pair (i_1,i_2) corresponds to Eqn. (3a) and Fig.1(a), or to Eqn.(3b) and Fig.1(b).

For the analogue of Eqn.(3a) as in Fig.1(a), we have

$$x_{i1} = (i_1-1)/I_1,\ x_{i2} = (i_2-1)/I_2,\ m_i = m(i_1,i_2),\ i=1 \text{ to } I_1I_2 \qquad (23a)$$

and similarly for the I'-grid. Then, we use (21a) unchanged, but change (21b) into (23b) as follows:

$$c_1(i_1-1)+1 = i'_1+i_{f1}\ ;\ c_2(i_2-1)+1 = i'_2+i_{f2} \qquad (23b)$$

Eqns. (22a-d) can then be applied unchanged to get the contributions from m_i in the I-grid to m'_i at four grid points of the I'-grid

For the analogue of Eqn.(3b) as in Fig.1(b), we have

$$x_{i1} = (i_1-\tfrac{1}{2})/I_1,\ x_{i2} = (i_2-\tfrac{1}{2})/I_2,\ m_i = m(i_1,i_2),\ i=1 \text{ to } I_1I_2 \qquad (24a)$$

and then Eqn. (21b) alone gets modified to (24b), as follows:

$$c_1(i_1-\tfrac{1}{2})+\tfrac{1}{2} = i'_1+i_{f1}\ ;\ c_2(i_2-\tfrac{1}{2})+\tfrac{1}{2} = i'_2+i_{f2} \qquad (24b)$$

and (22a-d) can be used without change.

It is to be noted that Fig.1(a), Eqn. (3a) and Eqns. (21), (23a-b), (22a-d), were used for the n.c.s. structure FSG-1 relevant to Tables 1-4 (for which the origin is immaterial). However, since an i-atom on a centre of symmetry is undesirable, Fig.1(b) and Eqn.(3b) are used for the grid approximation of the c.s. structure FSI2-1, whose data are given in Table 5 in section 4(e). When interpolation is performed for these I-coordinates, obviously, Eqns. (24a) and (24b) have to be employed with (22a-d) unchanged for calculating the interpolated m_i'-values.

(c) Minimum function calculations.

In Tables 2, 3 and 4, either 6X6 and 8X8 grid approximations have been obtained for the structure FSG2-1, with large temperature factors (K~10 to 15, B~1.26 to 0.84) corresponding to low resolution representations. An examination of these showed that the G-structures thus obtained are not superposable with the F-structure for comparison, because the origin can be taken at any point in a p1 unit cell. We considered various possible ways of verifying that a solution obtained for the F-structure does represent approximately the structure FSG-1 that is solved for (either in the real (crystal) space, or in the reciprocal (Fourier) space). The one that appeared most promising is the use of superposition methods - employing in particular the minimum-function integral to give an idea of the fit between the two structures. The relevant mathematics is briefly given below.

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Since each atom centred at (x_{j1},x_{j2}) has an electron density distribution $\rho_j(x_1,x_2) = (f_j/K)\exp\{-\pi K[(x_1-x_{j1})^2+(x_2-x_{j2})^2]\}$, the electron density, at (x_1,x_2) in the unit cell, is given by

$$\rho_F(x_1,x_2) = \sum_j (f_j/K)\exp\{-\pi K[(x_1-x_{j1})^2+(x_2-x_{j2})^2]\} \quad (25)$$

where the summation is to be performed over all atoms for which $l_j = [(x_1-x_{j1})^2+(x_2-x_{j2})^2]^{\frac{1}{2}} < l_o$, such that $\exp(-\pi K l_o^2)$ is greater than 0.005 (for example). This means that, for K~10 to 15, atoms outside the unit cell upto a distance of about 0.5 will have to be taken into account.

In the same way, for the approximate grid structure also, the e.d. function is:

$$\rho_G(x_1,x_2) = \sum_i (m_i/K)\exp\{-\pi K[(x_1-x_{i1})^2+(x_2-x_{i2})^2]\} \quad (26)$$

Then, we define the "minimum function", $\rho_{min}(x_1,x_2)$, as the lower of the two quantities $\rho_F(x_1,x_2)$ and $\rho_G(x_1,x_2)$. The minimum function is calculated at (x_{k1},x_{k2}) with $k_1 = 1$ to k_{1max}, $k_2 = 1$ to k_{2max} (for our studies k_{1max} is made equal to k_{2max} and a good value for this is 20.) Then, the "minimum function integral" (minint), approximated by the sum

$$\text{Minint} = \sum_{k_1=1}^{k_{1max}} \sum_{k_2=1}^{k_{2max}} \rho_{min}(x_{k1},x_{k2}); \quad k_1,k_2=1 \text{ to } 20 \quad (27)$$

gives the degree of superposition (DS) between the two structures ρ_F and ρ_G over the unit cell. The relevant equation is

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$$DS = Minint \; / \; F_{int} \qquad (28)$$

where

$$F_{int} = \sum_{k_1=1}^{k_{1max}} \sum_{k_2=1}^{k_{2max}} \rho_F(x_{k1},x_{k2}) = \sum_{J=1}^{J} f_j \qquad (29)$$

The value of DS is calculated for different shifts of origin, given by (x_{s1},x_{s2}) in the unit cell, and the maximum value of DS obtained therefrom is called "maximum degree of superposition" (MDS). Its value lies between 0.0 and 1.0, and gives a numerical estimate of the fit in electron density between the real structure $\rho_F(x_1,x_2)$ and the approximated grid structure $\rho_G(x_1,x_2)$, suitably shifted.

The check with various shifts for the origin is needed, since the origin can be chosen arbitrarily in the plane group p1. For the same reason, the handedness is also not fixed, and hence a second set of calculations from (26) to (28) will have to be done using the inverted G-structure ($\rho_G^!$), whose electron density is given by

$$\rho_G^!(x_1,x_2) = \rho_G(1-x_1,1-x_2), \quad x_1,x_2=0 \text{ to } 1 \qquad (30)$$

This gives a second value of MDS, namely MDS2 (calling the one obtained without inversion as MDS1). The higher of the two is chosen, and this gives the MDS of ρ_G with ρ_F.

This was tested, but an error was made in that atoms outside the unit cell were not included for calculating ρ_F and ρ_G. Hence the whole of the theory of this section has to be tested still.

..29

Also, practical procedures of mixing the information from 6X6, or 8X8, grid structures, obtained with different initial n.c.s. 4X4 grid structures have to be worked via minimum function methods.

(d) Centrosymmetric structures in plane group $p\bar{1}$.

All the above studies were made for a structure with plane group symmetry p1. To see as to how the theory works for a centrosymmetric structure, one example with the symmetry $p\bar{1}$ was examined. The structure chosen had 12 atoms in the asymmetric unit (j=1 to J/2). It was sought to be approximated by a 6X6 grid, having coordinates as in Eqn. (3b) and shown in Fig. 1(b). Only one half of the cell, with $0 \leqslant x_{i1} \leqslant \frac{1}{2}$ and $0 \leqslant x_{i2} < 1$ was used, and initial strengths m_i were fed in for 6X3 = 18 points in the half-cell. The refinement procedure was quite similar to that for p1 described in Section 2, the only difference being the changes in Eqns. (1) and (2b), which become

$$F(h_1,h_2) = 2\sum_{j=1}^{J/2} f_j \exp\left[-B(h_1^2+h_2^2)/4\right]\cos 2\pi(h_1x_{j1}+h_2x_{j2}) \qquad (31)$$

$$G(h_1,h_2) = 2\sum_{i=1}^{I/2} m_i \exp\left[-B(h_1^2+h_2^2)/4\right]\cos 2\pi(h_1x_{i1}+h_2x_{i2}) \qquad (32)$$

where

$$x_{i1} = (i_1-\tfrac{1}{2})/I_1 \quad , \quad x_{i2} = (i_2-\tfrac{1}{2})/I_2 \qquad (33)$$

As a consequence, Eqns. (12), (13), and (14) take the form

$$\sum_{i=1}^{I/2} p(H,i)\,\delta(i) = \Delta(H), \quad H=1 \text{ to } H_{max} \qquad (34)$$

..30

where

$$\Delta(H) = \Delta|F(H)| = (|F(H)| - |G(H)|) \; ; \; \delta(i) = \delta m_i \qquad (35a)$$

and

$$p(H,i) = \sum_{i=1}^{I/2} \frac{-\delta\Delta|F(H)|}{\delta m_i} = \sum_i T(H)\cos\theta(H,i)\,\mathrm{Sgn}(F(H)) \qquad (35b)$$

The rest of the equations from (14) to (19) are unchanged.

When this was applied with 18 m_i's to be determined, it was found that, with $H_1=H_2=5$ and $H_{max}=61$, the R-value came down from 1.3 to 0.25 in 10 cycles. The speed of convergence was <u>not much faster</u> than with 16 m_i's for the n.c.s. case. The print-out was so weak that full details could not be read out. Hence, they are not given. The case of $p\bar{1}$ symmetry requires further study.

<u>(e) Effect of fudge factor and errors</u>.

Random errors with mean values (e) 5%, 10% and 15% were introduced in $|F(H)|$ of 41 reflections forming one half of the set with $h_1, h_2 \leqslant 4$. So also, a fudge factor λ was introduced in Eqn.(16) to obtain m_i' from m_i and $\delta(i)$ as follows:

$$m_i' = m_i + \lambda\delta(i) \qquad (36)$$

With λ =1.0 and 1.5, using the diagonal approximations in the refinement, and using data with mean errors e as mentioned above, various combinations were tried, and the results indicated that errors upto 15% do not affect the final R-value very much. On the other hand, when the factor λ was made 1.5, the number of cycles to get the same R-value dropped by a factor of approximately 1.5. The data are summarized in Table 5.

Table 5: Effects of errors and fudge factor on the refinement procedure.

Table 5 : Effects of errors and fudge factor on the refinement procedure.*

Fudge factor λ	Mean error e	K = 10		K = 15	
		No.of iterations	R(final)	No.of iterations	R(final)
1.0	10	12	0.22	10	0.28
1.0	15	13	0.22	9	0.31
1.5	10	8	0.22	6	0.28
1.5	15	9	0.22	7	0.30

* Summarized from Output 79.

5. Extension to atoms with real form factors

(a) Gaussian atoms with corrected formulae including T(H)

In all the trials the correct structure was taken to be FSG-1 as given in Table 1(a) and the trial structure was GSG-7 given in the footnote of Table 4. When the diagonal approximation was used (output No. 90(d)), then for a 4X4 grid and K = 10 (B = 1.26) and using HMAX = 41, the R-values obtained for succeedir cycles were 0.561, 0.445, 0.269, 0.254. When the structure corresponding to the last value of R was interpolated to 5X5 and HMAX = 61 was used, on employing various values of K between 8 and 18, no refinement or convergence was achieved. In view of this when T(H) is included in the calculation, only the full matri: Gause-Seidel procedure was employed. However, it may be mentioned that when the fudge factor was made 0.5 and K was made equal to 20 (B = 0.63) for a 6X6 grid, the diagonal approximation led to a convergence from 0.544 to 0.241.

The results of refinement with the correct formula including T(H) and employing the Gause-Seidel full matrix calculations are summarized in Table 6.

Table 6: Results of refinement (with correct formula, including T(H).

Table 6. Results of Refinement
(With correct formula, including T(H))

Grid	K	B	HMAX	R-values
4X4	10	1.26	41	0.560 to 0.146
4X4	6	2.10	41	0.071, 0.066, 0.055
4X4	12	1.05	41	0.182,0.184,0.181,0.179
				After interpolation
6X6+	15	0.84	85	0.542, 0.455, 0.511,..
6X6+	12	1.05	85	0.435, 0.473, 0.477
6X6*	20	0.63	85	0.544 to 0.241
				Straight from random structure
6X6*	12	1.05	85	0.613, 0.303,..., 0.147

(+Fudge factor = 1.0; *Fudge factor = 0.5)

As will be seen from this, a range of values of K leads to refinement for the 4X4 grid while for the 6X6 grid only K = 20 (B = 0.63) led to convergence.

(b) Real crystals, with real atomic form factors

Since our technique is expected to work best for the case when all atoms are alike, the calculations were done only with all atoms having the form factor from a nitrogen atom which is given by

$$f_N(H) = 3.19 \exp(-(A/4)\, d^{*2}) + 2.31 \exp(-(A'/4)\, d^{*2}) + 1.50 \qquad (37)$$

$$A = 7.34, \quad A' = 26.8$$

This form factor is multiplied by an additional temperature factor which may be expressed by the function

$$T(H) = f(H) \exp\left\{-(B_T/4)\, d^{*2})\right]; \quad d^* = (2 \sin\theta)/\lambda \qquad (38$$

A suitable value of B_T is employed corresponding to the values of K and B used for gaussian atoms as given below in subsection (c). Thus, in these calculations employing a 3-dimensional crystal the inputs are a, b, c, α, β, γ, λ and from these we calculate $d(h_1,h_2,h_3)$ and $(\sin\theta)/\lambda = 1/2d = d^*/2$. The basic equations

are slightly modified, using this — e.g.

$$f(h_1,h_2,h_3) = \sum_{j=1}^{J} f_j(\sin\theta/\lambda)\exp\left[-BT(\sin\theta/\lambda)^2\right] x \exp 2\pi i(h_1x_{j1} + h_2x_{j2} + h_3x_{j3}) \quad (39)$$

Otherwise the function minimized is the same as before — namely R' given by

$$R' = \sum_{H} (|F(H)| - |G(H)|) = \sum_{H} \Delta|F(H)| \quad (40)$$

and the only change in the variation of $\Delta|F(H)|$ with m_i is the inclusion of f(H) and the use of new B_T's. We obtain

$$-\frac{\partial \Delta|F(H)|}{\partial m_i} = \frac{\partial |G(H)|}{\partial m_i} \quad 41$$

$$= f(H)\,T(H)\left\{C_c(H)\cos\theta(H,i) + C_s(H)\sin\theta(H,i)\right\}$$

(c) Test for a structure with nitrogen atoms

For comparison with the gaussian atom case, this was also tested with the structures FSG-1 and GSG-7, and a 4X4 grid, using, however, a square planar unit cell with a = 6Å, b = 6Å, $\gamma = 90^\circ$. Since the person who did these calculations could work only for two weeks at Bangalore, the program was tried only in four cases as given in Table 7.

Table 7. Refinement tests with nitrogen atoms

Table 7. Refinement tests with nitrogen atoms

(Unit cell a = 6Å, b = 6Å, Y = 90°)

FSG-1 and GSG-7; 4X4 grid

BT+	FF*	R-value variations	No. of cycles
70	1.0	0.66, 0.63, 0.57, 0.95**	—
70	0.5	0.623 to 0.193	13
50	0.5	0.738 to 0.179	20
40	0.5	0.778 to 0.183	19

+Temperature factor introduced for both S_F and S_G

*Fudge factor

**No refinement occurs.

Role of Fundamental Research in the Development of Technology

(Text of Keynote Address to be delivered at the Symposium on the occasion of the Post-Centenerary Silver Jubilee Celebrations of the University of Madras)

Matphil Reports No. 32, August 1983

Role of Fundamental Research in the Development of Technology

When Faraday was escorting a lady through his laboratori she asked him the question "What is the use of all these?" an it seems, he replied, "What is the use of a new born baby?" This strange reply of the great scientist was not a quip, but a very profound statement regarding the question that was rai Nobody can say what the new-born baby is going to be when he grows up; he may become a scientist, an author, a painter or great industrialist, but this cannot be discovered at the ti when he is born, but will become clear only as he grows up and his full potentialities are revealed. In the same way, a beautiful new phenomenon, which has been covered by a yo scientist, may not have in it any indication, at the time of its discovery, of what it is going to be 50 years or 100 year hence.

Considering Faraday's own great discovery of electromagn induction and the development of the theory of electricity a

magnetism and the interactions between the two, this was the result of pure curiosity on his part in trying to understand the phenomenon of electromagnetism. Within a very few years after that it had been converted into practical use, and it is not too much to say that our modern civilization is, to a large extent, dependent on electrical energy. The development of electrical technology could never have taken place if the fundamental basic laws were not put on firm grounds by Faraday a century ago. In fact, in 1931, the centenary of Faraday's discovery of electromagnetic induction was not conducted by the Royal Society of London, or the Royal Institution in London where he did all his studies, but by a technological Society — the Institution of Electrical Engineering, indicating that the applications of his discoveries in practical technology have far exceeded even the applications of his theories in basic physical sciences. But Faraday himself never bothered about these applications and he called himself only a "natural philosophe

magnetism and the interactions between the two, this was the result of pure curiosity on his part in trying to understand the phenomenon of electromagnetism. Within a very few years after that it had been converted into practical use, and it is not too much to say that our modern civilization is, to a large extent, dependent on electrical energy. The development of electrical technology could never have taken place if the fundamental basic laws were not put on firm grounds by Faraday a century ago. In fact, in 1931, the centenary of Faraday's discovery of electromagnetic induction was not conducted by the Royal Society of London, or the Royal Institution in London where he did all his studies, but by a technological Society — the Institution of Electrical Engineering, indicating that the applications of his discoveries in practical technology have far exceeded even the applications of his theories in basic physical sciences. But Faraday himself never bothered about these applications and he called himself only a "natural philosopher

It is strange that Faraday was not a mathematician and yet became a superb physicist discovering many new Laws of Nature. I am saying this in order to show that science is a field that is open to everybody, and to indicate that great discoveries are not made always as a result of intensive application and effort over a number of years, but quite often come in the form of sparks to the right person, who puts his mind in tune with nature, and tries to learn about the Laws of Nature.

It was in his attempt to translate Faraday's ideas into mathematical notation that Maxwell come out with his theory of electromagnetic waves. In fact, Maxwell's first paper was entitled "On Faraday's Lines of Force". Looking at these physical lines of force by his mental eye, Maxwell, who greatly abhorred the idea of action at a distance, postulated the existence of the electromagnetic field and worked out the laws governing the variations of the electric and magnetic field

vectors interacting one with the other, in the form of differential equations. In this way, he came to the well-known four Maxwell Equations, which, on further being manipulated by purely mathematical techniques, led to the prediction that there should occur electromagnetic waves emanating from systems in which the electric and magnetic field vary with time. Although the electromagnetic waves of Maxwell were actually discovered only some years later, Maxwell was fully convinced of the existence of these waves and even stated that it is a form of electromagnetic wave with transverse polarization.

We all know how Hertz produced these electromagnetic waves and studied them and how Marconi went ahead with the practical application of this new phenomenon and established that signals can be transmitted through vacuumn or over large distances in the atmosphere in the form of electromagnetic waves. I need not say anything about the technology of radio and wireless phenomena. They have completely engrossed everything in our daily life and

between the two, namely electromagnetic induction and electromagnetic waves, modern civilization is enveloped in every way by the applications that have come out of these purely scientific discoveries.

Now I shall pass on to another great discovery made in the 1850's but which found application only a century thereafter. This is the subject of Boolean algebra, developed by the mathematician-philosopher George Boole. He probed into the nature of science and wrote two books -- one on "Mathematical Analysis of Logic" (1847), and the other entitled "An Investigation of the Laws of Thought" (1854). In these books, he studied mathematically the nature of the qualitative relations between objects, phenomena etc., as contrasted with quantitative ones, which had been greatly studied by mathematicians of that time. In quality, he particularly emphasized the question — "Does a given quality belong to a given object or not?" The answer

is always either "yes" or "no", and he developed the algebra pertaining to such questions. There are only two possibilities to any mathematical entity in Boolean algebra and Boole expressed this by the arithematical symbols 1 and 0 — 1 for "yes" or truth, and 0 for "no" or falsity. With this, he built up a whole range of ideas by which mathematical thought and logical analysis can be converted into algebraic equations in Boolean algebra, and he used this for checking theories in logic.

Almost a century later, ideas of Boolean algebra began to be converted into practical things. It was Shannon who first showed that switching circuits had the property of simulating the 1-and-0 quality that was demanded by Boole. If a switch is on, the current exists and when it is off, the current goes away. Therefore "on" and "off" in a circuit can represent Boole's two entities 1 and 0. Also, two switches, in series and in parallel, can simulate the logical connectives "and" and "or" respectively. It was a very simple matter thereafter

to make larger and larger circuits to represent, by electrical signals, any analysis made by Boolean algebra, and practically exhibit the logical results thus obtained.

In the 1940's, these ideas found fruition in the development of the modern electronic computer. I shall not go into the details of this and the various improvements that were made — from the first computer ENIAC constructed in Princeton, to the enormously complicated and powerful computers of today. What is important to know is that the computer circuits are all based on the "all or nothing" nature of a quantity corresponding to 1 and 0 of Boolean algebra. Addition and multiplication in the binary system of arithematic can be represented by just these two signals, and it is a wonderful thing to know that modern computers can go through billions and trillions of operations of this kind without making a single error. The switching circuits constructed manually were replaced by integrated

circuits on chips and during the last two decades they have been replaced by large scale integrated circuits (LSI), and particularly during the last five years, by very large scale integrated circuits (VLSI). A VLSI is practically a computer by itself and can in a space of few milimeters cover what a room-full of electronic circuitry could do only thirty years ago.

In this revolution of computer technology, transistors have played a most fundamental part; and solid state physics, and the great developments that have taken place in this subject, have been fundamental for the great advances in the subject of computer science. Transistor technology is another example of pure basic research leading to a major technological advancement. We all know that transistors were not discovered as an attempt to find a new way of doing electrical technology. Rather they came as a result of the curiosity of scientists like Bardeen who tried to understand the phenomena in solid state in relation to the electrical properties of the materials. It is not a

surprising thing that the discovery of the transistor was made in the laboratories of Bell Telephones — a purely technological organization. However, it must be said that, in these laboratories, they allowed the scientists to pursue pure researc in whatever direction they desired, without any restraint on the nature, or financial outlay.

We may consider one more example, namely the discovery of radioactivity by becquerel and the Curies towards the end of the last century, which came about purely from an interest in studying fluorescent materials containing uranium and the origin of the light emission by these minerals. Such an innocent study has led to the development of the whole field of nuclear physics leading to the technological advance of obtaining energy from the atomic nucleus. These practical applications have had a tremendous impact on our lives all over the world.

I think it is not necessary to elsborate the point any further. We can say that, even in spite of the great advances in technology that have come in the 20th Century, the further advances or development of techniques both in technology and science are not going to be done merely by doing industrail research; but only from fundamental research. I believe, and I think it is generally accepted by all scientists, that significant advances are going to take place only by the lone scientist who sits in his laboratory pondering upon the laws of Nature and trying to discover new connections between them. It may be questioned whether scientists in a underdeveloped country like ours will be able to do anything in this direction without extremely well-equipped laboratories are available in the advanced countries of the west. The answer to this is that a really important discovery does not require very great facilities, but rather the application of the minds of scientists to probe into the secrets of nature and attempt to unravel these.

I think it will not be impertinent on my part if I pointed out how the discovery of the Raman Effect took place in India by Prof. Sir C.V. Raman using only very simple spectroscopic equipment which was available everywhere. Here again, this discovery has become a house-hold word in the laboratories of chemists, although it was a landmark in the development of pure physics in the subject of quantum theory, when it was discovered. Now-a-days the Raman Effect is applied for a whole variety of chemical investigations and a Laser Raman spectrograph is a must in every chemical laboratory — be it in a University, a Technological Institute or a technical laboratory.

In the same way as the Raman effect was found in India, there is every likelihood that new theoretical and experimental discoveries of an outstanding nature can come from this country, provided the scientists are given full freedom to work on whatever they like and utilize their time in research activities.

I feel that there is a greater chance of new and outstanding discoveries in the field of basic science taking place in India, rather than in applied and technological research. This is because of the reason I mentioned above, namely that discoveries in fundamental science are unpredictable and can occur to any good scientist who whole-heartedly applies himself to the pursuit of pure knowledge. What is needed is only to give a right atmosphere for such scientists to be free of worries and the need to waste their time in getting things done day-to-day, and allowing them to freely go ahead with their research activities. On the other hand, in technology, we have to first attain a high degree of competence before we obtain a new technological advance in our country. However, in the field of atomic energy and space research, our country has done absolutely first-class work, comparable to the best anywhere, as has been mentioned by the previous speakers.

This has been made possible by providing scientists working on these two disciplines full freedom from worry and ample financial and technological assistance at a high priority by our Government. The very fact that, as a consequence, the work done by these departments are comparable to the best in the world shows that the Indian scientists and particularly the younger generation of Indian scientists have the capability of doing absolutely top-class work, given the necessary facilitie

Unfortunately, this is not equally true of those who are working in pure research in Universities and related Institutes. If it is experimental research, then it is [illegible] facilities for this purpose, and only recently have our authorities woken up to the fact that the best facilities should be concentrated at specific places for each subject. Several such centres have been established during the last decade and if the development of activities in such centres

grows on and we are able to attract the best people from abroad to come and work in our country, then these laboratories will surely produce top rate fundamental work.

It is in the field of pure theory that it is a little difficult to understand why the output from India has not been commensurate with the quality that we expect from our scientists. The only explanation I can give is that spikes of achievement will occur only if the average base from which these spikes arise is itself high. Here it is that we are finding it difficult particularly during the last 20 or 30 years, to keep the best scientists in the country itself without allowing them to settle abroad. Always when such persons come back, they take three to four years to settle down, by which time they find themselves out of their depth in the competition with corresponding scientists abroad. But with the great stress on basic research that has been put by the Department of Science and Technology and the attempt to support especially active research workers

in selected thrust areas, it is very likely that a turn in the tide will take place in the next ten years or so, and that we can hope to talk of extremely high grade work being done in basic science in our research laboratories.

This is what should be done — not so much of large amounts of money being spread out everywhere, but rather of whatever we have being concentrated in a small number of places that have shown capabilities of producing high-class work and supporting the scientists there through the intervening period when they are keeping themselves settled and putting forward their ideas to producing high grade work. It is not an easy thing to say that a scientist is doing good work, when, in the meanwhile, he has not produced anything much but is striving towards perfection. It is the responsibility of the senior scientists of our country to pick out such persons who show promise of doing high grade scientific work although not actually producing

papers to justify that. It is necessary for such senior scientists, not to depend upon reports that are received from various laboratories, but instead visit the more promising laboratories all over the country, spend time with the younger scientists, talking to them and get to know what they are doing, what difficulties they are facing, and so on, and advise the Government suitably to support such persons. Such protective patronage by the senior scientists is the only thing that can give encouragement to the younger scientists when they are going through the process of trying to achieve something that is exceptionally good.

I am reminded in this connection of what Sir Lawrence Bragg, in the United Kingdom got a million pounds for a period of twenty years for the development of the subject of protein crystallography. Kendrew and Perutz who were selected by him to spearhead this project did not produce any papers for ten years or so, but Bragg was there to support them, and inform

the Medical Research Council, who supported their research, that work was going on and that it was going to be successful in the years to come. People of the stature of Brag are not many in India but those who are Advisers to the Department of Science and Technology should take this attitude and give impartial judgement of theirs on the activities of younger scientists in India. There should be something more than what is put on paper that should be taken into account in deciding who should be supported to the hilt, or we should be glad not to go ahead with his studies, even though he has not been sufficiently successful. If the younger scientists feel the existence of such support from the senior scientists and if that always goes to the right person in the right spirit, then I am sure more and more of the younger scientists will return to India and take part in our attempts to build up high quality basic research in the country.